Sphere Packings I

Thomas C. Hales

Abstract: We describe a program to prove the Kepler conjecture on sphere packings. We then carry out the first step of this program. Each packing determines a decomposition of space into Delaunay simplices, which are grouped together into finite configurations called Delaunay stars. A score, which is related to the density of packings, is assigned to each Delaunay star. We conjecture that the score of every Delaunay star is at most the score of the stars in the face-centered cubic and hexagonal close packings. This conjecture implies the Kepler conjecture. To complete the first step of the program, we show that every Delaunay star that satisfies a certain regularity condition satisfies the conjecture.

Contents: 1. Introduction, 2. The Program, 3. Quasi-regular Tetrahedra, 4. Quadrilaterals, 5. Restrictions, 6. Combinatorics, 7. The Method of Subdivision, 8. Explicit Formulas for Compression, Volume, and Angle, 9. Floating-Point Calculations.

Appendix. D. J. Muder's Proof of Theorem 6.1.

Section 1. Introduction

The Kepler conjecture asserts that no packing of spheres in three dimensions has density exceeding that of the face-centered cubic lattice packing. This density is $\pi/\sqrt{18} \approx 0.74048$. In an earlier paper [H2], we showed how to reduce the Kepler conjecture to a finite calculation. That paper also gave numerical evidence in support of the method and conjecture. This finite calculation is a series of optimization problems involving up to 53 spheres in an explicit compact region of Euclidean space. Computers have little difficulty in treating problems of this size numerically, but a naive attempt to make a thorough study of the possible arrangements of these spheres would quickly exhaust the world's computer resources.

The first purpose of this paper is to describe a program designed to give a rigorous proof of the Kepler conjecture. A sketch of a related program appears in [H2]. Although the approach of [H2] is based on substantial numerical evidence, some of the constructions of that paper are needlessly complicated. This paper streamlines some of those constructions and replaces others with constructions that are more

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amenable to rigorous methods. For this program to succeed, the original optimization problem must be partitioned into a series of much smaller problems that may be treated by current computer technology or hand calculation.

The second purpose of this paper is to carry out the first step of the proposed program. A statement of the result is contained in Theorem 1 below.

Background to another approach to this problem is found in [H3]. To add more detail to the proposed program, we recall some constructions from earlier papers [H1], [H2]. Begin with a packing of nonoverlapping spheres of radius 1 in Euclidean three-space. The *density* of a packing is defined in [H1]. It is defined as a limit of the ratio of the volume of the unit balls in a large region of space to the volume of the large region. The density of the packing may be improved by adding spheres until there is no further room to do so. The resulting packing is said to be *saturated*. It has the property that no point in space has distance greater than 2 from the center of some sphere.

Every saturated packing gives rise to a decomposition of space into simplices called the *Delaunay decomposition*. The vertices of each Delaunay simplex are centers of spheres of the packing. None of the centers of the spheres of the packing lie in the interior of the circumscribing sphere of any Delaunay simplex. In fact, this property is enough to completely determine the Delaunay decomposition except for certain degenerate packings. A degeneracy occurs, for instance, when two Delaunay simplices have the same circumscribing sphere. In practice, these degeneracies are important, because they occur in the face-centered cubic and hexagonal close packings. The paper [H2] shows how to resolve the degeneracies by taking a small perturbation of the packing. In general, the Delaunay decomposition will depend on this perturbation. We refer to the centers of the packing as *vertices*, since the structure of the simplicial decomposition of space will be our primary concern. For a proof that the Delaunay decomposition is a dissection of space into simplices, we refer the reader to [R].

The Delaunay decomposition is dual to the well-known Voronoi decomposition. If the vertices of the Delaunay simplices are in nondegenerate position, two vertices are joined by an edge exactly when the two corresponding Voronoi cells share a face, three vertices form a face exactly when the three Voronoi cells share an edge, and four vertices form a simplex exactly when the four corresponding Voronoi cells share a vertex. In other words, two vertices are joined by an edge if they lie on a sphere that does not contain any other of the vertices, and so forth (again assuming the vertices to be in nondegenerate position). The collection of all simplices that share a given vertex is called a *Delaunay star*. (This is a provisional definition: it will be refined below.)

Every Delaunay simplex has edges between 2 and 4 in length and, because of the saturation of the packing, a circumradius of at most 2. We assume that every

simplex S in this paper comes with a fixed order on its edges, $1, \ldots, 6$. The order on the edges is to be arranged so that the first, second, and third edges meet at a vertex. We may also assume that the edges numbered i and $i + 3$ are opposite edges for $i = 1, 2, 3$. We define $S(y_1, \ldots, y_6)$ to be the (ordered) simplex whose ith edge has length y_i. If S is a Delaunay simplex in a fixed Delaunay star, then it has a distinguished vertex, the vertex common to all simplices in the star. In this situation, we assume that the edges are numbered so that the first, second, and third edges meet at the distinguished vertex.

A function, known as the *compression* $\Gamma(S)$, is defined on the space of all Delaunay simplices. Let $\delta_{oct} = (-3\pi + 12\arccos(1/\sqrt{3}))/\sqrt{8} \approx 0.720903$ be the density of a regular octahedron with edges of length 2. That is, place a unit ball at each vertex of the octahedron, and let δ_{oct} be the ratio of the volume of the part of the balls in the octahedron to the volume of the octahedron. Let S be a Delaunay simplex. Let B be the union of four unit balls placed at each of the vertices of S. Define the compression as

$$\Gamma(S) = -\delta_{oct}\mathrm{vol}(S) + \mathrm{vol}(S \cap B).$$

We extend the definition of compression to Delaunay stars D^* by setting $\Gamma(D^*) = \sum \Gamma(S)$, with the sum running over all the Delaunay simplices in the star.

In this and subsequent work, we single out for special treatment the edges of length between 2 and 2.51. The constant 2.51 was determined experimentally to have a number of desirable properties. This constant will appear throughout the paper. We will call vertices that come within 2.51 of each other *close neighbors*.

We say that the convex hull of four vertices is a *quasi-regular tetrahedron* (or simply a *tetrahedron*) if all four vertices are close neighbors of one another. Suppose that we have a configuration of six vertices in bijection with the vertices of an octahedron with the property that two vertices are close neighbors if and only if the corresponding vertices of the octahedron are adjacent. Suppose further that exactly one of the three diagonals has length at most $2\sqrt{2}$. In this case we call the convex hull of the six vertices a *quasi-regular octahedron* (or simply an *octahedron*).

The compatibility of quasi-regular tetrahedra and octahedra with the Delaunay decomposition is established in Section 3. We think of Euclidean space as the union of quasi-regular tetrahedra, octahedra, and various less interesting Delaunay simplices. From now on, a Delaunay star is to be the collection of all quasi-regular tetrahedra, octahedra, and Delaunay simplices that share a common vertex v. This collection of Delaunay simplices and quasi-regular solids is often, but not always, the same as the objects called Delaunay stars in [H2]. We warn the reader of this shift in terminology.

It is convenient to measure the compression in multiples of the compression of the regular simplex of edge length 2. We define a *point* (abbreviated *pt*) to be $\Gamma(S(2,2,2,2,2,2))$. We have $pt = 11\pi/3 - 12\arccos(1/\sqrt{3}) \approx 0.0553736$.

One of the main purposes of this paper and its sequel is to replace the compression by a function (called the *score*) that has better properties than the compression. Further details on the definition of score will appear in Section 2. We are now able to state the main theorem of this paper.

Theorem 1. If a Delaunay star is composed entirely of quasi-regular tetrahedra, then its score is less than $8\,pt$.

The idea of the proof is the following. Consider the unit sphere whose center is the center of the Delaunay star D^*. The intersection of a simplex in D^* with this unit sphere is a spherical triangle. For example, a regular tetrahedron with edges of length 2 gives a triangle on the unit sphere of arc length $\pi/3$. The star D^* gives a triangulation of the unit sphere. The restriction on the lengths of the edges of a quasi-regular tetrahedron constrains the triangles in the triangulation. We classify all triangulations that potentially come from a star scoring more than $8\,pt$. Section 5 develops a long list of properties that must be satisfied by the triangulation of a high-scoring star.

It is then necessary to classify all the triangulations that possess the properties on this list. The original classification was carried out by a computer program, which generated all potential triangulations and checked them against the list. D. J. Muder has made a significant improvement in the argument by giving a direct, computer-free classification. His result appears in the appendix.

As it turns out, there is only one triangulation that satisfies all of the properties on the list. Section 7 proves that Delaunay stars with this triangulation score less than $8\,pt$. This will complete the main thread of the argument.

There are a number of estimates in this paper that are established by computer. These estimates are used throughout the paper, even though their proofs are not discussed until Sections 8 and 9. These sections may be viewed as a series of technical appendices giving explicit formulas for the compression, dihedral angles, solid angles, volumes, and other quantities that must be estimated. The final section states the inequalities and gives details about the computerized verification. There is no vicious circle here: the results of Sections 8 and 9 do not rely on anything from Sections 2–7.

There are several functions of a Delaunay simplex that will be used throughout this

defined to be the dihedral angle of the simplex S along the first edge (with respect to the fixed order on the edges of S). Set $\mathrm{dih}_{\min} = \mathrm{dih}(S(2, 2, 2.51, 2, 2, 2.51)) \approx 0.8639$; $\mathrm{dih}_{\max} = \mathrm{dih}(S(2.51, 2, 2, 2.51, 2, 2)) = \arccos(-29003/96999) \approx 1.874444$. We will see that $\mathrm{dih}_{\min}$ and $\mathrm{dih}_{\max}$ are lower and upper bounds on the dihedral angles of quasi-regular tetrahedra. The *solid angle* (measured in steradians) at the vertex joining the first, second, and third edges is denoted $\mathrm{sol}(S)$. The intersection of S with the ball of unit radius centered at this vertex has volume $\mathrm{sol}(S)/3$ (see [H1,2.1]). For example, $\mathrm{sol}(S(2, 2, 2, 2, 2, 2)) \approx 0.55$. Let $\mathrm{rad}(S)$ be the circumradius of the simplex S. In Section 2, we will define two other functions: $\mathrm{vor}(S)$, which is related to the volume of Voronoi cells, and the score $\sigma(S)$. Finally, let $\eta(a, b, c)$ denote the circumradius of a triangle with edges a, b, c. Explicit formulas for all these functions appear in Section 8.

Section 2. The Program

By proving Theorem 1, the main purpose of this paper will be achieved. Nevertheless, it might be helpful to give a series of comments about how Theorem 1 may be viewed as the solution to the first of a handful of optimization problems that would collectively provide a solution to the Kepler conjecture.

We begin with some notation and terminology. We fix a Delaunay star D^* about a vertex v_0, which we take to be the origin, and we consider the unit sphere at v_0. Let v_1 and v_2 be vertices of D^* such that v_0, v_1, and v_2 are all close neighbors of one another. We take the radial projections p_i of v_i to the unit sphere with center at the origin and connect the points p_1 and p_2 by a geodesic arc on the sphere. We mark all such arcs on the unit sphere. Lemma 3.10 will show that the arcs meet only at their endpoints. The closures of the connected components of the complement of these arcs are regions on the unit sphere, called the *standard regions*. We may remove the arcs that do not bound one of the regions. The resulting system of edges and regions will be referred to as the *standard decomposition* of the unit sphere.

Let C be the cone with vertex v_0 over one of the standard regions. The collection of the Delaunay simplices, quasi-regular tetrahedra, and quasi-regular octahedra of D^* in C (together with the distinguished vertex v_0) will be called a *standard cluster*. Each Delaunay simplex in D^* belongs to a unique standard cluster. Each triangle in the standard decomposition of the unit sphere is associated with a unique quasi-regular tetrahedron, and each tetrahedron determines a triangle in the standard decomposition (Lemma 3.7). We may identify quasi-regular tetrahedra with clusters over triangular regions.

We assign a score to each standard cluster in [H4,3]. In this section we define the score of a quasi-regular tetrahedron and describe the properties that the score should have in general.

Let S be a quasi-regular tetrahedron. It is a standard cluster in a Delaunay star with center v_0. If the circumradius of S is at most 1.41, then we define the score to be $\Gamma(S)$.

If the circumradius is greater than 1.41, then embed the simplex S in Euclidean three-space. Partition Euclidean space into four infinite regions (infinite Voronoi cells) by associating with each vertex of S the points of space closest to that vertex. By intersecting S with each of the four regions, we partition S into four pieces $\hat{S}_0$, $\hat{S}_1$, $\hat{S}_2$, and $\hat{S}_3$, corresponding to its four vertices v_0, v_1, v_2, and v_3. Let sol_i be the solid angle at the vertex v_i of the simplex. The expression $-4\delta_{oct}\text{vol}(\hat{S}_0) + 4\,\text{sol}_0\,/3$ is an analytic function of the lengths of the edges for simplices S that contain their circumcenters. (Explicit formulas appear in Section 8.) This function may be analytically continued to a function of the lengths of the edges for simplices S that do not necessarily contain their circumcenters. Let $\text{vor}(S)$ be defined as the analytic continuation of $-4\delta_{oct}\text{vol}(\hat{S}_0) + 4\,\text{sol}_0\,/3$.

In this case, define the score of S to be $\text{vor}(S)$. Write $\sigma(S)$ for the score of a quasi-regular tetrahedron. In summary, the score is

$$\sigma(S) = \begin{cases} \Gamma(S), & \text{if the circumradius of } S \text{ is at most } 1.41, \\ \text{vor}(S), & \text{otherwise.} \end{cases}$$

The quasi-regular tetrahedron S appears in four Delaunay stars. In the other three Delaunay stars, the distinguished vertices will be v_1, v_2, and v_3, so that S, viewed as a standard cluster in the other Delaunay stars, will have scores $-\delta_{oct}\text{vol}(\hat{S}_i)+\text{sol}_i\,/3$ (or their analytic continuations), for $i = 1, 2, 3$. By definition,

$$\Gamma(S) = \sum_{i=0}^{3}(-\delta_{oct}\text{vol}(\hat{S}_i) + \text{sol}_i\,/3).$$

The sum of the scores of S, for each of the four vertices of S, is $4\Gamma(S)$. This is the same total that is obtained by summing the compression of S at each of its vertices. This is the property we need to relate the score to the density of the packing. It means that although the score reapportions the compression among neighboring Delaunay stars, the average of the compression over a large region of space equals the average of the score over the same region, up to a negligible boundary term.

The analytic continuation in the definition of $\text{vor}(S)$ has the following geometric interpretation. If the circumcenter of a quasi-regular tetrahedron S is not contained in S, a small tip of the infinite Voronoi cell at v_0 (or some other vertex) will protrude through the opposite face of the Delaunay simplex. The volume of this small protruding tip is not counted in $-4\delta_{oct}\text{vol}(\hat{S}_0) + 4\,\text{sol}_0\,/3$, but it is counted in the analytic continuation. The analytic continuations of the scores of S for each of the other three vertices acquire a term representing the negative volume of a part

of the tip. The three parts together constitute the entire tip, so that the negative volumes exactly offset the volume of the tip, and the sum of the four scores of S is $4\Gamma(S)$. Details appear in [H4].

The general definition of the score will have similar properties. To each standard cluster of a Delaunay star D^* a score will be assigned. The rough idea is to let the score of a simplex in a cluster be the compression $\Gamma(S)$ if the circumradius of every face of S is small, and otherwise to let the score be defined by Voronoi cells (in a way that generalizes the definition for quasi-regular tetrahedra).

The score $\sigma(D^*)$ of a Delaunay star is defined as the sum of the scores of its standard clusters. The score has the following properties [H4,3.1 and 3.5].

1. The score of a standard cluster depends only on the cluster, and not on the way it sits in a Delaunay star or in the Delaunay decomposition of space.

2. The Delaunay stars of the face-centered cubic and hexagonal close packings score exactly $8\,pt$.

3. The score is asymptotic to the compression over large regions of space. We make this more precise. Let Λ denote the vertices of a saturated packing. Let Λ_N denote the vertices inside the ball of radius N. (Fix a center.) Let $D^*(v)$ denote the Delaunay star at $v \in \Lambda$. Then the score satisfies (in Landau's notation)

$$\sum_{\Lambda_N} \sigma(D^*(v)) = \sum_{\Lambda_N} \Gamma(D^*(v)) + O(N^2).$$

Lemma 2.1. If the score of every Delaunay star in a saturated packing is at most $s < 16\pi/3$, then the density of the packing is at most $16\pi\delta_{oct}/(16\pi - 3s)$. If the score of every Delaunay star in a packing is at most $8\,pt$, then the density of the packing is at most $\pi/\sqrt{18}$.

Proof: The second claim is the special case $s = 8\,pt$. The proof relies on property 3. The number of vertices such that $D^*(v)$ meets the boundary of the ball B_N of radius N has order $O(N^2)$. Since the Delaunay stars give a four-fold cover of $\mathbb{R}^3$, we have

$$4(-\delta_{oct}\mathrm{vol}(B_N) + |\Lambda_N|\frac{4\pi}{3}) = \sum_{\Lambda_N}(-\delta_{oct}\mathrm{vol}(D^*(v)) + 4\,\mathrm{sol}(D^*(v))/3) + O(N^2)$$

$$= \sum_{\Lambda_N}\Gamma(D^*(v)) + O(N^2)$$

$$= \sum_{\Lambda_N}\sigma(D^*(v)) + O(N^2)$$

$$\leq s|\Lambda_N| + O(N^2).$$

Rearranging, we get

$$\frac{4\pi|\Lambda_N|}{3\text{vol}(B_N)} \le \frac{\delta_{oct}}{(1 - 3s/16\pi)} + \frac{O(N^2)}{\text{vol}(B_N)}.$$

In the limit, the left-hand side is the density and the right-hand side is the bound. Similar arguments can be found in [H1] and [H2]. ∎

The following conjecture is fundamental. By the lemma, this conjecture implies the Kepler conjecture. The lemma also shows that weaker bounds than $8\,pt$ on the score might be used to give new upper bounds on the density of sphere packings.

Conjecture 2.2. The score of every Delaunay star is at most $8\,pt$.

The basic philosophy behind the approach of this paper is that quasi-regular tetrahedra are the only clusters that give a positive score, standard clusters over quadrilateral regions should be the only other clusters that may give a score of zero, and every other standard cluster should give a negative score. Moreover, we will prove that no quasi-regular tetrahedron gives more than $1\,pt$.

Thus, heuristically, we try to obtain a high score by including as many triangular regions as possible. If we allow any other shape, preference should be given to quadrilaterals. Any other shape of region should be avoided if possible. If these other regions occur, they should be accompanied by additional triangular regions to compensate for the negative score of the region. We will see later in this paper that even triangular regions tend to give a low score unless they are arranged to give five triangles around each vertex.

The main steps in a proof of the Kepler conjecture are

1. *A proof that even if all regions are triangular the total score is less than $8\,pt$*

2. *A proof that standard clusters in regions of more than three sides score at most $0\,pt$*

3. *A proof that if all of the standard regions are triangles or quadrilaterals, then the total score is less than $8\,pt$ (excluding the case of pentagonal prisms)*

4. *A proof that if some standard region has more than four sides, then the star scores less than $8\,pt$*

5. *A proof that pentagonal prisms score less than $8\,pt$*

The division of the problem into these steps is quite arbitrary. They were originally intended to be steps of roughly equal magnitude, although is has turned out that a construction in [H4] has made the second step substantially easier than the long calculations of the third step.

This paper carries out the first step. The second step of the program is also complete [H4]. Partial results are known for the third step [H5]. In the fourth step, it will be necessary to argue that these regions take up too much space, give too little in return, and have such strongly incompatible shapes that they cannot be part of a winning strategy.

To make step 5 precise, we define *pentagonal prisms* to be Delaunay stars whose standard decomposition has ten triangles and five quadrilaterals, with the five quadrilaterals in a band around the equator, capped on both ends by five triangles (Diagram 2.3.) The conjecture in this section asserts, in particular, that pentagonal prisms, which created such difficulties in [H2], score less than $8\,pt$. The final step has been separated from the third step, because the estimates are expected to be more delicate for pentagonal prisms than for a general Delaunay star in the third step.

Diagram 2.3
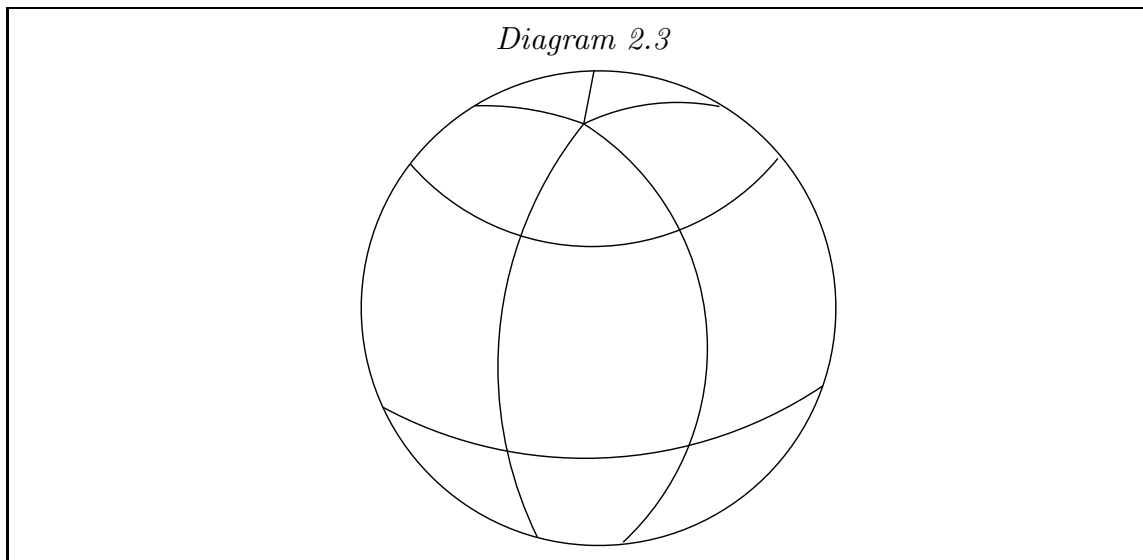
One of the main shortcomings of the compression is that pentagonal prisms have compression greater than $8\,pt$ (see [H2]). Numerical evidence suggests that the upper bound on the compression is attained by a pentagonal prism, denoted D^*_{ppdp} in [H2], at about $8.156\,pt$, and this means that the link between the compression and the Kepler conjecture is indirect. The score appears to correct this shortcoming.

What evidence is there for the conjecture and program? They come as the result of extensive computer experimentation. I have checked the conjecture against much of the data obtained in the numerical studies of [H2,9.3]. The data suggest that the score tends to give a dramatic improvement over the compression, often improving

the bound by more than a point. The score of the particularly troublesome pentagonal prism D^*_{ppdp} drops safely under $8\,pt$. I have checked a broad assortment of other pentagonal prisms and have found them all to score less than $8\,pt$.

The second step shows that no serious pathologies can arise. The only way to form a Delaunay star with a positive score is by arranging a number of quasi-regular tetrahedra around a vertex (together with other standard clusters that can only lower the score). There must be at least eight tetrahedra to score $8\,pt$, and if there are any distortions in these tetrahedra, there must be at least nine. However, as this paper shows, too many quasi-regular tetrahedra in any star are also harmful. Future papers will impose additional limits on the structure of the optimal Delaunay star.

Section 3. Quasi-Regular Tetrahedra

This section studies the compatibility of the Delaunay simplices and the quasi-regular solids. Fix three vertices v_1, v_2, and v_3 that are close neighbors to one another. Let T be the triangle with vertices v_i. It does not follow that T is the face of a Delaunay simplex. However, as we will see, when T is not the face of a simplex, the arrangement of the surrounding simplices is almost completely determined.

If T is not the face of a Delaunay simplex, then we will show that there are two additional vertices v_0 and v_0', where v_0 and v_0' are close neighbors to v_1, v_2, and v_3. This means that there are two quasi-regular tetrahedra S_1 and S_2 with vertices (v_0, v_1, v_2, v_3) and (v_0', v_1, v_2, v_3), respectively, that have the common face T (see Diagram 3.1.a). We will see that $S_1 \cup S_2$ is the union of three Delaunay simplices with vertices (v_0, v_0', v_1, v_2), (v_0, v_0', v_2, v_3), and (v_0, v_0', v_3, v_1) in Diagram 3.1.b. This section establishes that this is the only situation in which quasi-regular tetrahedra are not Delaunay simplices: they must come in pairs and their union must be three Delaunay simplices joined along a common edge. The decomposition of this paper is obtained by taking each such triple of Delaunay simplices (3.1.b) and replacing the triple by a pair of quasi-regular tetrahedra (3.1.a).

Diagram 3.1
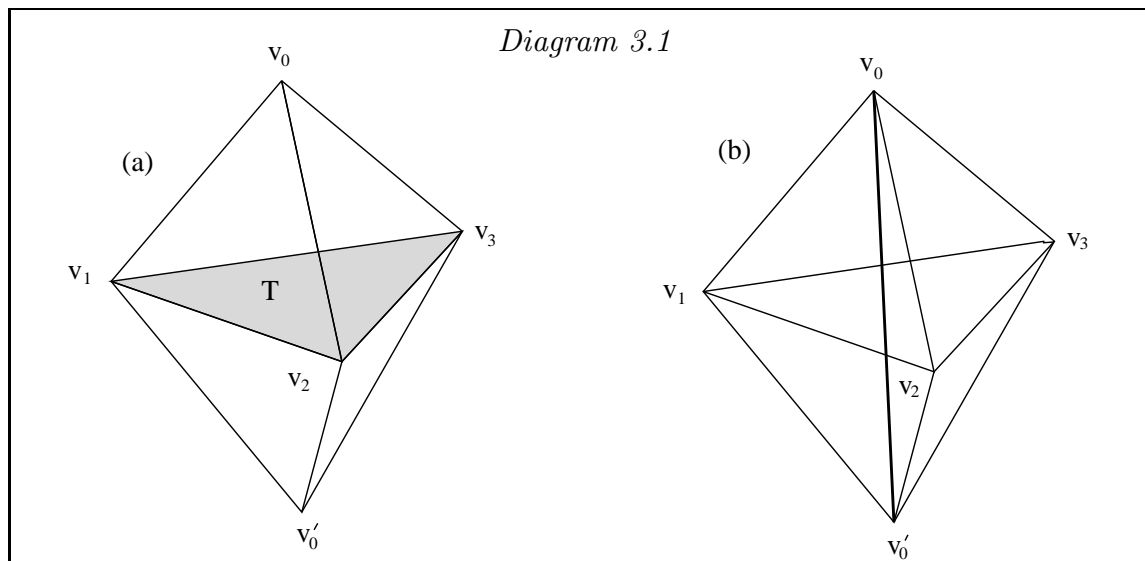
From the dual perspective of Voronoi cells, the Voronoi cell at v_0 (or v_0') would have a small tip protruding from S_1 through T, if the vertex v_0' were not present. The vertex v_0' slices off this protruding tip so that the Voronoi cells at v_0 and v_0' have a small face in common.

Lemma 3.2. Suppose that the circumradius of the triangle T is less than $\sqrt{2}$. Then T is the face of a Delaunay simplex.

Proof: Let $r < \sqrt{2}$ be the radius of the circle that circumscribes T, and let c be the center of the circle. The sphere of radius r at c does not contain any vertices of D^* other than v_1, v_2, and v_3. By the definition of the Delaunay decomposition (as described in the introduction), this implies that T is the face of a simplex. ∎

Remark 3.3. We have several constraints on the edge lengths, if T is not a face of a Delaunay simplex. Consider the circumradius $\eta(a, b, c)$ of a triangle whose edges have lengths a, b, c between 2 and 2.51. Since $2.51^2 < 2^2+2^2$, we see that the triangle is acute, so that $\eta(a, b, c)$ is monotonically increasing in a, b, and c. This gives simple estimates relating the circumradius to a, b, and c. The circumradius is at most $\eta(2.51, 2.51, 2.51) = 2.51/\sqrt{3} \approx 1.449$. If the circumradius is at least $\sqrt{2} \approx 1.41421$, then a, b, and c are greater than 2.3 ($\eta(2.3, 2.51, 2.51) \approx 1.41191 < \sqrt{2}$). Under the same hypothesis, two of a, b, and c are greater than 2.41 ($\eta(2.41, 2.41, 2.51) < \sqrt{2}$). Finally, at least one edge has length greater than 2.44 ($\eta(2.44, 2.44, 2.44) < \sqrt{2}$).

Lemma 3.4. Let T be the triangle with vertices v_i. Assume that the vertices v_i are close neighbors of one another. Suppose there is a vertex v_0 that lies closer to the circumcenter of T than the vertices of T do. Then the vertex v_0 satisfies

$2 \leq |v_0 - v_i| < 2.15$, for $i = 1, 2, 3$. In particular, the convex hull of $v_0, \ldots, v_3$ is a quasi-regular tetrahedron S with face T.

Another way of stating the hypothesis on the circumcenter is to say that the plane of T separates v_0 from the circumcenter of S. Because of the constraints on the edge lengths in Remark 3.3, the three other faces of S are faces of Delaunay simplices.

Proof: We defer the proof to Section 8.2.5. ∎

Lemma 3.5. Let v, v_1, v_2, v_3, and v_4 be distinct vertices with pairwise distances at least 2. Suppose that the pairs (v_i, v_j) are close neighbors for $\{i, j\} \neq \{1, 4\}$. Then v does not lies in the convex hull of (v_1, v_2, v_3, v_4).

Proof: For a contradiction, suppose v lies in the convex hull. Since $|v - v_i| \geq 2$ and for $\{i, j\} \neq \{1, 4\}$, v_i and v_j are close neighbors, the angle formed by v_i and v_j at the vertex v is at most $\theta_0 = \arccos(1 - 2.51^2/8) \approx 1.357$. Each such pair of vertices gives a geodesic arc of length at most θ_0 radians on the unit sphere centered at v. We obtain in this way a triangulation of the unit sphere by four triangles, two with edges of length at most $\theta_0 = 2\arcsin(2.51/4)$ radians, and two others that fit together to form a quadrilateral with edges of at most θ_0 radians. By the spherical law of cosines, the area formula for a spherical triangle, and [H2,6.1], each of the first two triangles has area at most $3\arccos(\cos\theta_0/(1 + \cos\theta_0)) - \pi \approx 1.04$. By the same lemma, the quadrilateral has area at most the area of a regular quadrilateral of side θ_0, or about 2.8. Since the combined area of the two triangles and quadrilateral is less than 4π, they cannot give the desired triangulation. To see that v cannot lie on the boundary, it is enough to check that a triangle having two edges of lengths between 2 and 2.51 cannot contain a point that has distance 2 or more from each vertex. We leave this as an exercise. ∎

Corollary 3.5.1 No vertex of the packing is ever an interior point of a quasi-regular tetrahedron or octahedron.

Proof: The corollary is immediate for a tetrahedron. For an octahedron, draw the distinguished diagonal and apply the lemma to each of the four resulting simplices. ∎

Let T be a triangle of circumradius between $\sqrt{2}$ and $2.51/\sqrt{3}$, with edges of length between 2 and 2.51. Consider the line through the circumcenter of T, perpendicular

circumcenters of the two simplices with face T formed by placing an additional vertex at distance two from the three vertices of of T on either side of the plane through T.

Lemma 3.6. Let S be a simplex formed by the vertices of T and a fourth vertex v_0'. Suppose that the circumcenter of S lies on the segment s. Assume that v_0' has distance at least 2 from each of the vertices of T. Then v_0' has distance less than 2.3 from each of the vertices of T.

Proof: Let v_1, v_2, v_3 be the vertices of T. For a contradiction, assume that v_0' has distance at least 2.3 from a vertex v_1 of T. Lemma 3.4 shows that the plane through T does not separate v_0' from the circumcenter of S. If the circumcenter lies in s (and is not separated from v_0' by the plane through T), then by moving v_0' to decrease the circumradius, the circumcenter remains in s.

Let S be the simplex with vertices v_0', v_1, v_2, and v_3. The circumcenter of S lies in the interior of S. We omit the proof, because it is established by methods similar to (but longer than) the proof of Lemma 3.4. Thus, the circumradius is increasing in the lengths of $|v_0' - v_i|$, for $i = 1, 2, 3$ (see 8.2.4).

Let R be the circumradius of a simplex with face T and center an endpoint of s. We will prove that the circumradius of S is greater than R, contrary to our hypothesis. Moving v_0' to decrease the circumradius, we may take the distances to v_i to be precisely 2.3, 2, and 2. We may move v_1, v_2, and v_3 along their fixed circumscribing circle until $|v_2 - v_3| = 2.51$ and $|v_1 - v_2| = |v_1 - v_3|$ in a way that does not decrease any of the distances from v_0' to v_i. Repeating the previous step, we may retain our assumption that v_0' has distances exactly 2.3, 2, and 2 from the vertices v_i as before. We have reduced the problem to a one-dimensional family of tetrahedra parametrized by the radius r of the circumscribing circle of T. Set $x(r) = |v_1 - v_3| = |v_2 - v_3|$. To obtain our desired contradiction, we must show that the circumradius $R'(r)$ of the simplex $S(2.3, 2, 2, 2.51, x(r), x(r))$ satisfies $R'(r) > R(r)$. Since both R' and R are increasing in r, for $r \in [\sqrt{2}, 2.51/\sqrt{3}]$, the desired inequality follows if we evaluate the 200 constants

$$R'(r_i) - R(r_{i+1}), \qquad \text{for } r_i = \sqrt{2} + \left(\frac{2.51}{\sqrt{3}} - \sqrt{2} \right) \frac{i}{200},$$

for $i = 0, \dots, 199$, and check that they are all positive. (The smallest is about 0.00005799, which occurs for $i = 199$.) ∎

Let T be a triangle made up of three close neighbors. Suppose that T is not the face of a Delaunay simplex. There exists a vertex v_0 whose distance to the circumcenter of T is less than the circumradius of T. Let S be the quasi-regular tetrahedron formed by v_0 and the vertices of T. It is not a Delaunay simplex, so there exists

a vertex v_0' that is less than the circumradius of S from the circumcenter of S. Let S' be the simplex formed by v_0' and the vertices of T. It is not a Delaunay simplex either. The circumcenter of S lies in the segment s of Lemma 3.4, so the circumcenter of S' does too. The lengths of the edges of S and S' other than T are constrained by Lemmas 3.4 and 3.6. In particular, in light of Remark 3.3, the faces other than T of S and S' are faces of Delaunay simplices.

If v_0 and v_0' lie on the same side of the plane through T, then either v_0' lies in S, v_0 lies in S', or the faces of S and S' intersect nonsimplicially. None of these situations can occur because a nondegenerate Delaunay decomposition is a Euclidean simplicial complex and because of Lemma 3.5. We conclude that v_0 and v_0' lie on opposite sides of the plane through T.

$S \cup S'$ is bounded by Delaunay faces, so $S \cup S'$ is a union of Delaunay simplices. The fourth vertex of the Delaunay simplex in $S \cup S'$ with face (v_0, v_1, v_2) cannot be v_3 (S is not a Delaunay simplex), so it must be v_0'. Similarly, (v_0, v_0', v_2, v_3) and (v_0, v_0', v_3, v_1) are Delaunay simplices. These three Delaunay simplices cannot be quasi-regular tetrahedra by Lemma 8.3.2.

The assumption that T is not a face has completely determined the surrounding geometry: there are two quasi-regular tetrahedra S and S' along T such that $S \cup S'$ is a union of three Delaunay simplices.

Lemma 3.7. Let L be a union of standard regions. Suppose that the boundary of L consists of three edges. Then either L or its complement is a single triangle.

For example, the interior of L cannot have the form of Diagram 3.8. Lemma 3.5 (proof) shows that if all regions are triangles, then there are at least 12 triangles, so that the exterior of L cannot have the form of Diagram 3.8 either.

Diagram 3.8
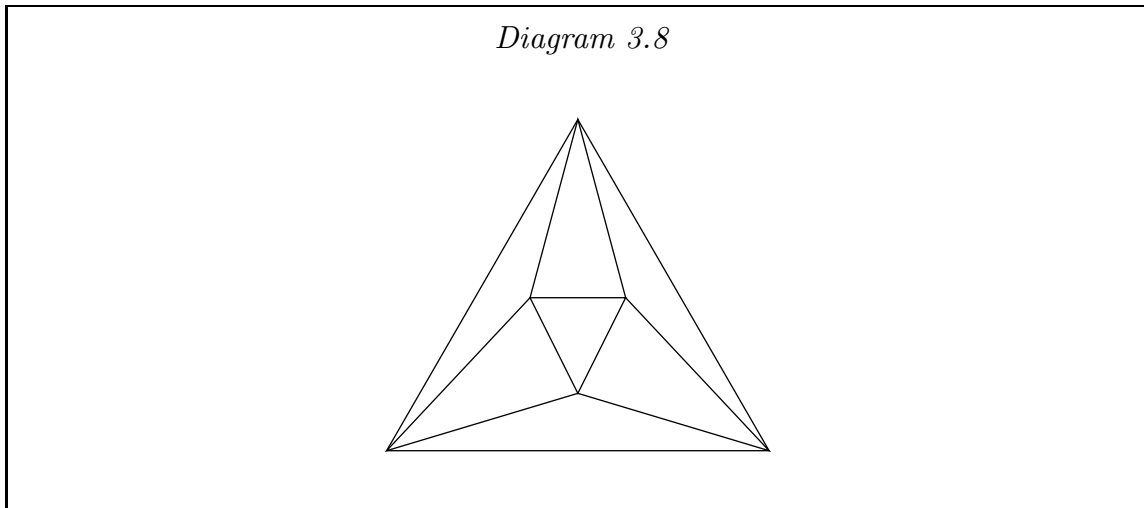
Proof: Replacing L by its complement if necessary, we may assume that the area of L is less than its complement. The triangular boundary corresponds to four vertices v_0 (the origin), v_1, v_2, and v_3. The close-neighbor constraints on the lengths show that the convex hull of $v_0, \ldots, v_3$ is a quasi-regular tetrahedron. By construction each quasi-regular tetrahedron is a single cluster. ∎

We say that a point $v \in \mathbb{R}^3$ is *enclosed* by a region on the unit sphere if the interior of the cone (with vertex v_0) over that region contains v. For example, in Diagram 3.9, the point v is enclosed by the given spherical triangle.

Diagram 3.9
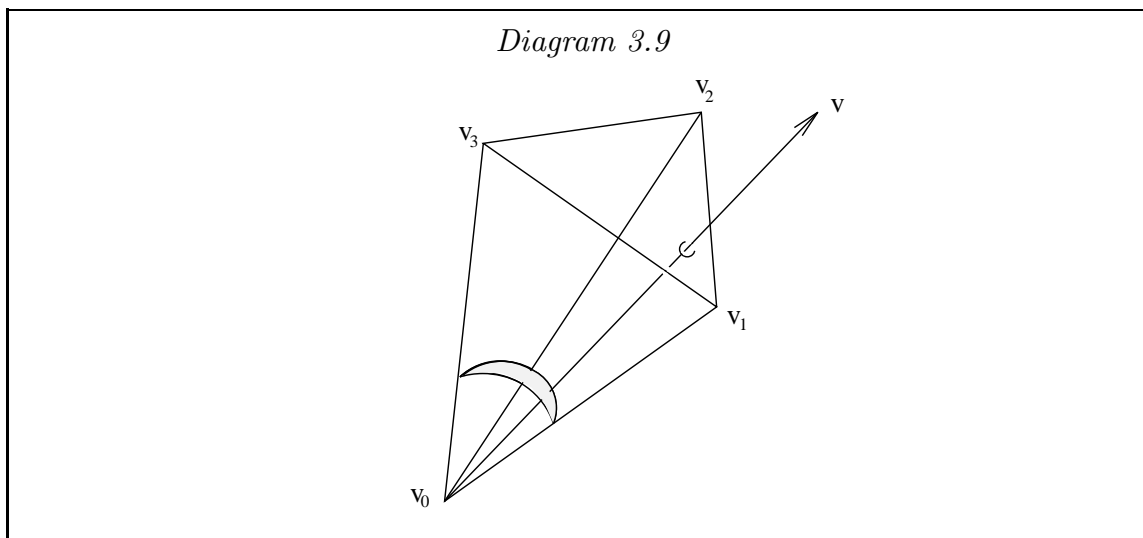
The following lemma was used in Section 2 to define the standard decomposition.

Lemma 3.10. Fix a Delaunay star D^* with center v_0. Draw geodesic arcs on the unit sphere at v_0 for every triple of close neighbors v_0, v_1, v_2 (as in Section 2). The resulting system of arcs do not meet except at endpoints.

Proof. Our proof will be based on the fact that a nondegenerate Delaunay decomposition is a Euclidean simplicial complex. Let T_1 and T_2 be two triangles made from two such triples of close neighbors. We have $T_i \subset S_i \cup S_i'$, where S_i and S_i are the Delaunay simplices with face T_i if T_i is the face of a Delaunay simplex, and they are the two quasi-regular tetrahedra with face T_i constructed above, otherwise. Since a nondegenerate Delaunay decomposition is a Euclidean simplicial complex, $S_1 \cup S_1'$ meets $S_2 \cup S_2'$ simplicially. By the restrictions on the lengths of the edges in Lemmas 3.4 and 3.6, this forces T_1 to intersect T_2 simplicially. The result follows. ∎

Section 4. Quadrilaterals

Fix a Delaunay star composed entirely of quasi-regular tetrahedra and consider the

by four edges of the triangulation. L will be the union of two or more triangles. Replacing L by its complement in the unit sphere if necessary, we assume that the area of L is less than that of its complement.

We claim that in this context, L is the union of either two or four triangles, as illustrated in Diagram 4.1. In particular, L encloses at most one vertex. If a diagonal to the quadrilateral L is an edge of the triangulation, the region L is divided into two triangles each associated with a quasi-regular tetrahedron. In particular, there is no enclosed vertex. (Lemma 3.7 precludes any subtriangulation of a triangular region.) If, however, there is a single enclosed vertex and neither diagonal is an edge of the triangulation, then the only possible triangulation of L is the one of the diagram. Proposition 4.2 completes the proof of the claim.

Diagram 4.1
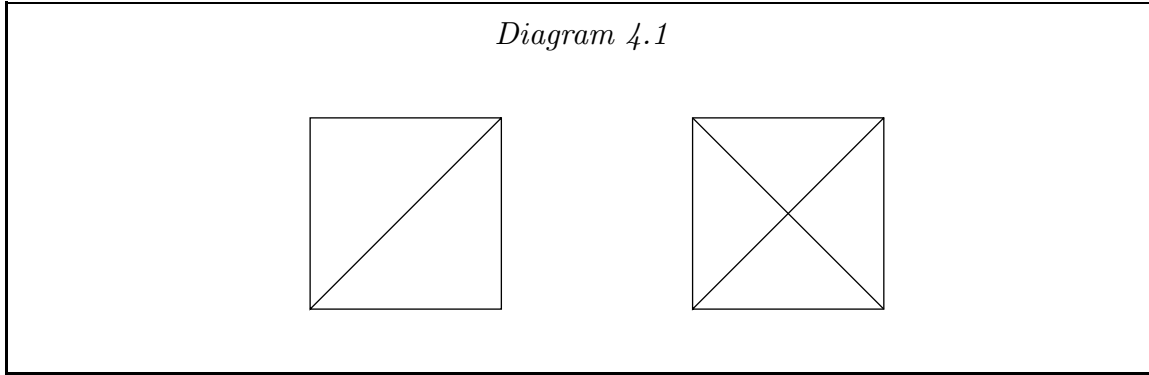
Proposition 4.2. A union of regions (of area less than 2π) bounded by exactly four edges cannot enclose two vertices of distance at most 2.51 from the origin.

This argument is somewhat delicate: if our parameter 2.51 had been set at 2.541, for instance, such an arrangement would exist. First we prove a useful reduction.

Lemma 4.3. Assume a figure exists with vectors $v_1, \ldots, v_4$, v, and v' subject to the constraints

$$2 \leq |v_i| \leq 2.51,$$
$$2 \leq |v_i - v_{i+1}| \leq k_i,$$
$$2 \leq |v_i - v_{i+2}|,$$
$$2 \leq |v - v'|,$$
$$h_i \leq |w - v_i|,$$
$$2 \leq |w| \leq \ell, \text{ for } w = v, v' \text{ and } i = 1, \ldots, 4 \ (\text{mod} 4)$$

where ℓ, h_i, and k_i are fixed constants that satisfy $\ell \in [2.51, 2\sqrt{2}]$, $h_i \in [2, 2\sqrt{2})$, $k_i \in [2, 2.51]$. Let L be the quadrilateral on the unit sphere with vertices $v_i/|v_i|$ and edges running between consecutive vertices. Assume that v and v' lie in the cone at the origin obtained by scaling L. Then another figure exists made of a (new) collection of vectors $v_1, \ldots, v_4$, v, and v' subject to the constraints above together with the additional constraints

$$|v_i - v_{i+1}| = k_i$$
$$|v_i| = 2, \text{ for } i = 1, \ldots, 4,$$
$$|v| = |v'| = \ell.$$

Moreover, the quadrilateral L may be assumed to be convex.

Proof (4.3): By rescaling v and v', we may assume that $|v| = |v'| = \ell$. (Moving v or v' away from the origin increases its distance from the other vertices of the configuration.)

The diagonals satisfy $|v_2 - v_4| > 2.1$ and $|v_1 - v_3| > 2.1$. Otherwise, if say $|v_1 - v_3| \leq 2.1$, then the faces with vertices (v_1, v_2, v_3) and (v_1, v_4, v_3) have circumradius less than $\sqrt{2}$. The edge from 0 to v has length at most $\sqrt{2}$, so this edge cannot intersect these faces by the Euclidean simplicial complex argument used before 3.7 and in 3.10. By Lemma 3.5, v cannot lie in the convex hull of $(0, v_1, v_3, v_i)$. This leaves v nowhere to go, and a figure with $|v_1 - v_3| \leq 2.1$ does not exist.

Next, we claim that we may assume that the quadrilateral L is convex (in the sense that it contains the geodesic arcs between any two points in the region). To see this, suppose the vertex v_i lies in the cone over the convex hull of the other three vertices v_j. Consider the plane P through the origin, v_{i-1}, and v_{i+1}. The reflection v_i' of v_i through P is no closer to v, v', or v_{i+2} and has the same distance to the origin, v_{i-1}, and v_{i+1}. Thus, replacing v_i with v_i' if necessary, we may assume that L is convex.

Most of the remaining deformations will be described as pivots. We will fix an axis and rotate a vertex around a circle centered along and perpendicular to the given axis. If, for example, $|v_3 - v_4| < k_3$, we pivot the vertex v_4 around the axis through 0 and v_1 until $|v_3 - v_4| = k_3$. It follows from the choice of axes that the distances from v_4 to the origin and v_1 are left unchanged, and it follows from the convexity of L that $|w - v_4|$ increases for $w = v_2$, v_3, v, and v'. Similarly, we may pivot vertices v_i along the axis through the origin and v_{i+1} until $|v_i - v_{i-1}| = k_i$, for all i .

Fix an axis through two opposite vertices (say v_1 and v_3) and pivot another vertex (say v_2) around the axis toward the origin. We wish to continue by picking different axes and pivoting until $|v_i| = 2$, for $i = 1, 2, 3, 4$. However, this process appears to

vertices and the pivot toward the origin moves v_i closer to that enclosed vector. We must check that this situation can be avoided.

Interchanging the roles of (v_1, v_3) with (v_2, v_4) as necessary, we continue to pivot until $|v_1| = |v_3| = 2$ or $|v_2| = |v_4| = 2$ (say the former). We claim that either v_2 has distance greater than h_2 from v or that pivoting v_2 around the axis through v_1 and v_3 moves v_2 away from v. If not, we find that $|v_1| = |v_3| = 2$, $|v - v_2| = h_2$ and that v lies in the cone $C = C(v_2)$ with vertex v_2 spanned by the vectors from v_2 to the origin, v_1, and v_3. (This relies on the convexity of the region L.)

To complete the proof, we show that this figure made from $(0, v_1, v_2, v_3, v)$ cannot exist. Contract the edge (v, v_2) as much as possible keeping the triangle $(0, v_1, v_3)$ fixed, subject to the constraints that $v \in C(v_2)$ and $|w - w'| \geq 2$, for $w = v, v_2$ and $w' = 0, v_1, v_3$. This contraction gives $|v - v_2| \leq h_2 < 2\sqrt{2}$.

Case 1: v lies in the plane of $(0, v_2, v_3)$. This gives an impossibility: crossing edges (v, v_2) $(0, v_3)$ of length less than $2\sqrt{2}$. Similarly, v cannot lie in the plane of $(0, v_1, v_2)$.

Case 2: v lies in the interior of the cone $C(v_2)$. The contraction gives $|v - w'| = 2$ for $w = v, v_2$ and $w' = 0, v_1, v_3$. The edge (v, v_2) divides the convex hull of $(0, v_1, v_2, v_3, v)$ into three simplices. Consider the dihedral angles of these simplices along this edge. The dihedral angle of the simplex (v_1, v_2, v_3, v) is less than π. The dihedral angles of the other two are less than $\mathrm{dih}(S(2\sqrt{2}, 2, 2, 2, 2, 2)) = \pi/2$. Hence, the dihedral angles along the diagonal cannot sum to 2π and the figure does not exist.

Case 3: v lies in the plane of (v_2, v_1, v_3). Let r be the radius of the circle in this plane passing through v_1 and v_3 obtained by intersecting the plane with a sphere of radius 2 at the origin. We have $2r \geq |v_1 - v_3| > 2\sqrt{2}$ because otherwise we have the impossible situation of crossing edges (v_1, v_3) and (v_2, v) of length less than $2\sqrt{2}$. Let H be the perpendicular bisector of the segment (v_1, v_3). By reflecting v through H if necessary we may assume that v and v_2 lie on the same side of H, say the side of v_3. Furthermore, by contracting (v, v_2), we may assume without loss of generality that $|v_3 - v| = |v_2 - v_3| = 2$. Let $f(r) = |v - v_2|$, as a function of r. f is increasing in r. The inequalities $2\sqrt{2} > h_2 \geq |v - v_2| \geq f(\sqrt{2}) = 2\sqrt{2}$ give the desired contradiction. ∎

Proof (4.2): Assume for a contradiction that v and v' are vertices enclosed by L. Let the center of the Delaunay star be at the origin, and let $v_1, \ldots, v_4$, indexed consecutively, be the four vertices of the Delaunay star that determine the extreme points of L.

We will describe a sequence of deformations of the configuration (formed by the vertices $v_1, \ldots, v_4, v, v'$) that transform the original configuration of vertices into particular rigid arrangements below. We will show that these rigid arrangements cannot exist, and from this it will follow that the original configuration does not exist either. These deformations will preserve the constraints of the problem. To be explicit, we assume that that $2 \leq |w| \leq 2.51$, that $2 \leq |w - v_i|$ if $w \neq v_i$, that $2 \leq |v - v'|$, and that $|v_i - v_{i+1}| \leq 2.51$, for $i = 1, 2, 3, 4$ and $w = v_1, \ldots, v_4, v, v'$. Here and elsewhere we take our subscripts modulo 4, so that $v_1 = v_5$, and so forth. The deformations will also keep v and v' in the cone at the origin that is determined by the vertices v_i.

We consider some deformations that increase $|v - v'|$. By Lemma 4.3, we may assume that $|v_i| = 2$, $|v| = |v'| = |v_i - v_{i+1}| = 2.51$, for $i = 1, 2, 3, 4$. If, for some i, we have $|v_i - v| > 2$ and $|v_i - v'| > 2$, then we fix v_{i-1} and v_{i+2} and pivot v_{i+1} around the axis through the origin and v_{i+2} away from v and v'. The constraints $|v_{i+1} - v_i| = |v_i - v_{i-1}| = 2.51$ will force us to drag v_i to a new position on the sphere of radius 2. By making this pivot sufficiently small, we may assume that $|v_i - w|$ and $|v_{i+1} - w|$, for $w = v, v'$, are greater than 2.

The vertices v and v' cannot both have distance 2 from both v_{i+2} and v_{i-1}, for then we would have $v = v'$. So one of them, say v, has distance exactly 2 from at most one of v_{i+2} and v_{i-1} (say v_{i+2}). Thus, v may be pivoted around the axis through the origin and v_{i+2} away from v'. In this way, we increase $|v - v'|$ until $|v_i - v| = 2$ or $|v_i - v'| = 2$, for $i = 1, 2, 3, 4$.

Suppose one of v, v' (say v) has distance 2 from v_i, v_{i+1}, and v_{i+2}. The configuration is completely rigid. By symmetry, the vertices v_{i-1} and v' must be the reflections of v_{i+1} and v, respectively, through the plane through 0, v_i, and v_{i+2}. In particular, v' has distance 2 from v_i, v_{i-1}, and v_{i+2}. We pick coordinates and evaluate the length $|v - v'|$. We find that $|v - v'| \approx 1.746$, contrary to the hypothesis that the centers of the spheres of our packing are separated by distances of at least 2. Thus, the hypothesis that v has distance two from three other vertices is incorrect.
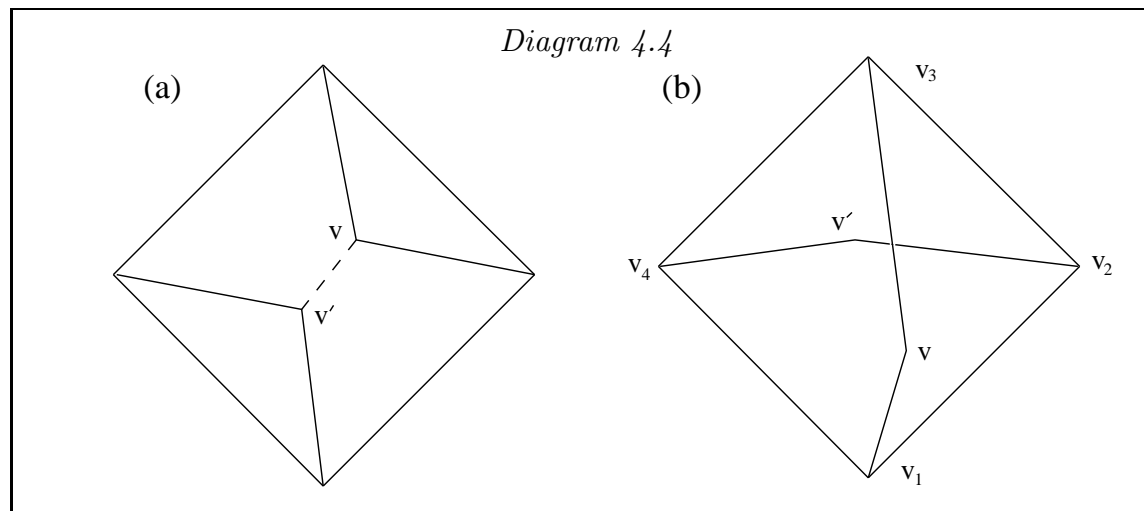
Diagram 4.4

We are left with one of the configurations of Diagram 4.4. An edge is drawn in the diagram, when the distance between the two endpoints has the smallest possible value (that is, 2.51 for the four edges of the quadrilateral, and 2 for the remaining edges). Deform the figure of case (a) along the one remaining degree of freedom until $|v - v'| = 2$. In case (a), referring to the notation established by Diagram 4.5, we have a quadrilateral on the unit sphere of edges $t_1 = 2\arcsin(2.51/4) \approx 1.357$ radians, $t_2 = \arccos(2.51/4)$ radians, and $t_3 = 2\arcsin(1/2.51)$ radians. The form of this quadrilateral is determined by the angle α, and it is clear that the angle $\beta(\alpha)$ is decreasing in α. We have

$$\theta = \mathrm{dih}_{\max} = \mathrm{dih}(S(2.51, 2, 2, 2.51, 2, 2)) \approx 1.874444.$$

The figure exists if and only if there exists α such that $\beta(\alpha) + \beta(2\pi - \theta - \alpha) = 2\pi - \theta$. By symmetry, we may assume that $\alpha \leq \pi - \theta/2 \approx 2.20437$. The condition $|v - v_1| \geq 2$ implies that

$$\alpha \geq \arccos\left((\cos t_2 - \cos t_2 \cos t_3)/(\sin t_2 \sin t_3)\right) > 1.21.$$

However, by monotonicity,

$$\beta(\alpha) + \beta(2\pi - \theta - \alpha) < \beta(\alpha_i) + \beta(2\pi - \theta - \alpha_i - 0.1) < 2\pi - \theta,$$

for $\alpha_i \leq \alpha \leq 0.1 + \alpha_i$, with $\alpha_i = 1.21 + 0.1\,i$, and $i = 0, 1, \ldots, 9$, as a direct calculation of the constants $\beta(\alpha_i) + \beta(2\pi - \theta - \alpha_i - 0.1)$ will reveal. (The largest constant, which is about $2\pi - \theta - 0.113$, occurs for $i = 0$.) Hence, the figure of Diagram 4.4.a does not exist.
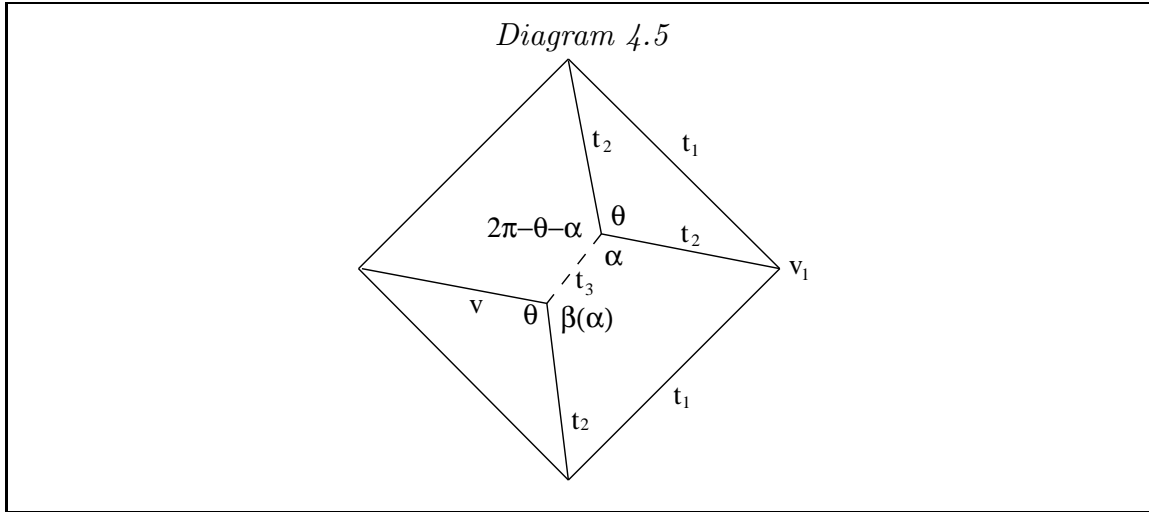
Diagram 4.5

To rule out Diagram 4.4.b, we reflect v, if necessary, to its image through the plane P through $(0, v_1, v_3)$, so that P separates v and v'. The vertex v can then be pivoted away from v' along the axis through v_1 and v_3. This decreases $|v|$, but we may rescale so that $|v| = 2.51$. Eventually $|v - v_2| = 2$ or $|v - v_4| = 2$. This is the previously considered case in which v has distance 2 from three of the vertices

v_i. This completes the proof that the original arrangement of two enclosed vertices does not exist. ∎

Section 5. Restrictions

If a Delaunay star D^* is composed entirely of tetrahedra, then we obtain a triangulation of the unit sphere. As explained in Section 2, we wish to prove that no matter what the triangulation is, we always obtain a score less than $8\,pt$. In this section we make a long list of properties that a configuration must have if it is to have a score of $8\,pt$ or more. The next section and the appendix show that only one triangulation satisfies all of these properties. Additional arguments will show that this triangulation scores less than $8\,pt$. This will complete the proof of Theorem 1.

In this section, the term *vertices* refers to the vertices of the triangulation of the unit sphere. The edges of the triangulation give a planar graph. We adopt the standard terminology of graph theory to describe the triangulation. We will speak of the degree of a vertex, adjacent vertices, and so forth. The n triangles around a vertex will be referred to as an n-gon. We will also refer to the corresponding n tetrahedra that give the triangles of the polygon. We say that a triangulation contains a *pattern* $(a_1, \dots, a_n)$, for $a_i \in \mathbb{N}$, if there are distinct vertices v_i of degrees a_i that are pairwise nonadjacent, for $i = 1, \dots, n$. Let N be the number of vertices in the triangulation, and let N_i be the number of vertices of degree i. We have $N = \sum N_i$.

In this section, we will start to use various inequalities from Section 9 related to the score. Since the score $\sigma(S)$ may be either $\Gamma(S)$ or $\mathrm{vor}(S)$ depending on the circumradius of S, there are two cases to consider for every inequality. In general, the inequalities for $\Gamma(S)$ are more difficult to establish. In the following sections, we will only cite the inequalities pertaining to $\Gamma(S)$. Section 9 shows how all the same inequalities hold for $\mathrm{vor}(S)$.

Proposition 5.1. Consider a Delaunay star D^* that is composed entirely of quasi-regular tetrahedra. Suppose that $\sigma(D^*) \geq 8\,pt$. Then the following restrictions hold on the triangulation of the unit sphere given by the standard decomposition.

1. $13 \leq N \leq 15$.

2. $N = N_4 + N_5 + N_6$.

3. A region bounded by three edges is either a single triangle or the complement of a single triangle.

4. Two degree four vertices cannot be adjacent.

5. $N_4 \leq 2$.

6. Patterns $(6, 6, 6)$ and $(6, 6, 4)$ do not exist.

7. The pattern $(6, 6)$ or $(6, 4, 4)$ implies that $N \geq 14$.

8. If there are two adjacent degree six vertices, and a third degree six vertex adjacent to neither of the first two, then $N = 15$ and all other vertices are adjacent to at least one of these three.

9. The triangulation is made of geodesic arcs on the sphere whose radian lengths are between 0.8 and 1.36.

Lemma 5.2. Consider a vertex of degree n, for some $4 \leq n \leq 7$. Let $S_1, \ldots, S_n$ be the tetrahedra that give the n triangles. Then $\sum_{i=1}^n \sigma(S_i)$ is less than z_n, where $z_4 = 0.33\,pt$, $z_5 = 4.52\,pt$, $z_6 = -1.52\,pt$, and $z_7 = -8.9\,pt$. Suppose that $n \geq 6$. Let $S_1, \ldots, S_4$ be any four of the n tetrahedra around the vertex. Then $\sum_{i=1}^4 \sigma(S_i) < 1.5\,pt$.

Proof (5.2): When $n = 4$, this is Lemma 9.5. When $n = 5$, this is Lemma 9.6. When $n = 6$ or $n = 7$, we have by Calculation 9.4

$$\sum_{i=1}^n \sigma(S_i) < \sum_{i=1}^n (0.378979\,\mathrm{dih}(S_i) - 0.410894)$$
$$= 2\pi(0.378979) - 0.410894n.$$

The right-hand side evaluates to about $-1.520014\,pt$ and $-8.940403\,pt$, respectively, when $n = 6$ and $n = 7$.

Assume that $n \geq 6$, and select any four $S_1, \ldots, S_4$ of the n tetrahedra around the vertex. Let S_5 and S_6 be two other tetrahedra around the vertex. The dihedral angles of S_5 and S_6 are are at least $\mathrm{dih}_{\min}$, by Calculation 9.3. Each of the four triangles (associated with $S_1, \ldots, S_4$) must then, on average, have an angle at most $(2\pi - 2\,\mathrm{dih}_{\min})/4$ at v. By Calculation 9.4,

$$\sum_{i=1}^4 \sigma(S_i) < \sum_{i=1}^4 (0.378979\,\mathrm{dih}(S_i) - 0.410894)$$
$$\leq (2\pi - 2\,\mathrm{dih}_{\min})0.378979 + 4(-0.410894) < 1.5\,pt.$$

∎

Proof (5.1): Let $t = 2(N - 2)$ be the number of triangles, an even number. By Euler's theorem on polyhedra,

$$3N_3 + 2N_4 + N_5 + 0N_6 - N_7 \cdots = 12.$$

Let $S_1, \ldots, S_t$ denote the tetrahedra of D^*. Let $\sigma_i = \sigma(S_i)$ be the corresponding

4π. Often, without warning, we will rearrange the indices i so that the tetrahedra that give the triangles around a given vertex are numbered consecutively. When a vertex v of the triangulation has been fixed, we will let α_i denote the angles of the triangles at v, so that $\sum \alpha_i = 2\pi$. The angle α_i of a triangle is equal to the corresponding dihedral angle of the simplex S_i. We abbreviate certain sums over n elements to $\sum_{(n)}$, when the context makes the indexing set clear. Throughout the argument, we will use Calculation 9.1, which asserts that $\sigma_i \leq 1\,pt$, for all i. The proofs will show that if a triangulation fails to have any of the properties 1–9, then the total score must be less than $8\,pt$.

(Proof of 5.1.1): Assume that $t \geq 28$. By Calculation 9.9,

$$\sum_{(t)} \sigma_i < \sum_{(t)} (0.446634\,\mathrm{sol}_i - 0.190249) \leq 4\pi(0.446634) + t(-0.190249)$$

$$\leq 4\pi(0.446634) + 28(-0.190249) \leq 8\,pt.$$

Suppose that $t \leq 18$. By Calculation 9.8,

$$\sum_{(t)} \sigma_i < \sum_{(t)} (-0.37642101\,\mathrm{sol}_i + 0.287389) = 4\pi(-0.37642101) + t(0.287389)$$

$$\leq 4\pi(-0.37642101) + 18(0.287389) \leq 8\,pt.$$

This proves that $12 \leq N \leq 15$. The case $N = 12$ will be excluded after 5.1.2.

(Proof of 5.1.2): By Lemma 8.3.2 and Calculation 9.3, each angle α of each triangle satisfies $\mathrm{dih}_{\min} \leq \alpha \leq \mathrm{dih}_{\max}$. In particular, $\alpha > \pi/4$, so that each vertex has degree less than eight, and $\alpha < 2\pi/3$, so that each vertex has degree greater than three.

Assume for a contradiction that there is a vertex of degree seven. Consider the seven tetrahedra around the given vertex. By Lemma 5.2, the tetrahedra satisfy

$$\sum_{(7)} \sigma_i < -8.9\,pt.$$

Suppose $t \leq 24$. For each vertex v, set $\zeta_v = \sum_v \sigma_i$, the sum running over the tetrahedra around v. Clearly, $\sum_{(t)} \sigma_i = (\sum_v \zeta_v)/3$. Pick a vertex v that is not a vertex of any of the seven triangles of the heptagon. By Lemma 5.2, we see that $\zeta_v < 0.33\,pt$ if v has degree four, $\zeta_v < 4.52\,pt$ if v has degree five, $\zeta_v < -1.52\,pt$ if v has degree six, and $\zeta_v < -8.9\,pt$ if v has degree seven. In particular, if v has degree n, then ζ_v falls short of n points by at least $0.48\,pt$. Thus,

$$\sum_{(t)} \sigma_i < \sum_{(7)} \sigma_i + \sum_{(t-7)} pt - 0.48\,pt \leq (-8.9 + (24 - 7) - 0.48)\,pt < 8\,pt.$$

Finally, we assume that $t = 26$ and $N = 15$. If $N_6 = 0$ and $N_7 = 1$, then Euler's theorem gives the incompatible conditions $2N_4 + N_5 - 1 = 12$ and $N_4 + N_5 + 1 = 15$. Thus, $N_6 > 0$ or $N_7 > 1$. This gives a second k-gon ($k = 6$ or 7) around a vertex v. This second polygon shares at most two triangles with the original heptagon. This leaves at least four triangles of a second polygon exterior to the first. Thus, by Lemma 5.2,

$$\sum_{(26)} \sigma_i \leq \sum_{(7)} \sigma_i + \sum_{(4)} \sigma_i + \sum_{(t-11)} pt < -8.9\,pt + 1.5\,pt + (26 - 11)\,pt < 8\,pt.$$

(Proof of 5.1.1, cont.): Assume $N = 12$. We define three classes of quasi-regular tetrahedra. In the first class, all the edges have lengths between 2 and 2.1. In the second, the fourth, fifth, and sixth edges have lengths greater than 2.1. The third class is everything else.

Set $\epsilon = 0.001$, $a = -0.419351$, $b = 0.2856354$. The following are established by Calculations 9.10 – 9.12.

$$\sigma(S) \leq a\,\mathrm{sol}(S) + b + \epsilon, \quad \text{for } S \text{ in the first class,}$$
$$\sigma(S) \leq a\,\mathrm{sol}(S) + b, \quad \text{for } S \text{ in the second class,}$$
$$\sigma(S) \leq a\,\mathrm{sol}(S) + b - 5\epsilon, \quad \text{for } S \text{ in the third class,}$$

Consider a vertex v of degree $n = 4$, 5, or 6 and the surrounding tetrahedra $S_1, \ldots, S_n$. We claim that

(5.1.1.1)
$$\sum_{i=1}^{n} \sigma(S_i) \leq \sum_{i=1}^{n} (a\,\mathrm{sol}(S_i) + b).$$

This follows directly from the stated inequalities if none of these tetrahedra are in the first class. It is also obvious if at least one of these tetrahedra is in the third class, because then the inequality is violated by at most $-5\epsilon + (n - 1)\epsilon \leq 0$. So assume that all of the tetrahedra are in the first two classes with at least one in the first class. By the restrictions on the lengths of the edges, a tetrahedron in the first class cannot be adjacent to one in the second class. We conclude that the tetrahedra are all in the first class.

By Lemma 5.2, $z_n \leq n(0.904)pt$. If $\sum_{(n)} \mathrm{sol}(S_i) \leq n(0.56176)$, then

$$\sum_{(n)} \sigma(S_i) \leq n(0.904)\,pt \leq \sum_{(n)} (a(0.56176) + b) \leq \sum_{(n)} (a\,\mathrm{sol}(S_i) + b).$$

So we may assume that $\sum_{(n)} \mathrm{sol}(S_i) \geq n(0.56176)$. By Calculation 9.13,

$$\sum_{(n)} \sigma(S_i) \leq \sum_{(n)} (-0.65557\,\mathrm{sol}(S_i) + 0.418)$$

$$\leq \sum (a\,\mathrm{sol}(S_i) + b) + \sum (0.132365 - 0.236219(0.56176)) < \sum (a\,\mathrm{sol}(S_i) + b).$$

This establishes inequality 5.1.1.1. By averaging over every vertex, we see that the average of the scores $\sigma(S)$ is less than the average of $a\,\mathrm{sol}(S) + b$. So

$$\sigma(D^*) = \sum_{(t)} \sigma(S) \le \sum_{(t)} (a\,\mathrm{sol}(S) + b) = 4\pi a + 20b \approx 7.99998\,pt < 8\,pt.$$

(Proof of 5.1.3): This is Lemma 3.7. (If we had not introduced quasi-regular tetrahedra, then this result would no longer hold.)

(Proof of 5.1.4): If two degree four vertices are adjacent, we then have the arrangement of Diagram 5.3. This is a quadrilateral enclosing two vertices, contrary to Proposition 4.2.

Diagram 5.3
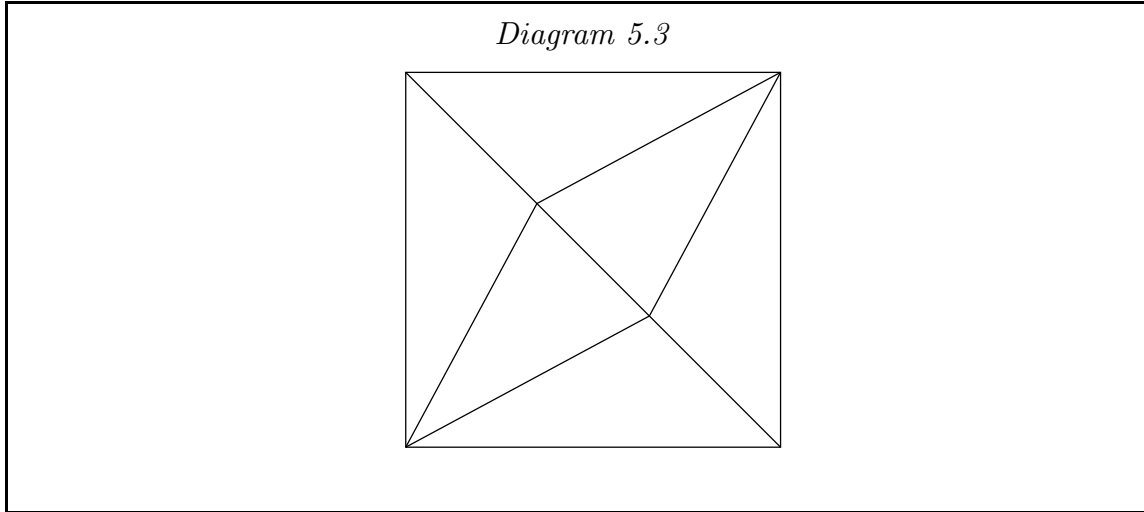
(Proof of 5.1.5): As in the proof of 5.1.2, for each vertex v, set $\zeta_v = \sum_v \sigma_i$, the sum running over the tetrahedra around the vertex v. We use the estimates of ζ_v that appear in Lemma 5.2.

We have found that $N_i = 0$, if $i \ne 4, 5, 6$. By Euler's theorem, $N_5 = 12 - 2N_4$ and $N_6 = N_4 + N - 12$. Assume that $N \ge 13$ and that $N_4 \ge 3$. Then

$$\sum_{(t)} \sigma_i = \frac{1}{3}\sum_{(N)} \zeta_v < \frac{1}{3}(0.33N_4 + 4.52(12 - 2N_4) - 1.52(N_4 + N - 12))\,pt$$

$$\le \frac{1}{3}(0.33(3) + 4.52(12 - 6) - 1.52(3 + 13 - 12))\,pt < 8\,pt.$$

(Proof of 5.1.6): Suppose that we have the pattern $(6, 6, 6)$. Then reordering indices according to the polygons in the pattern, we have by the estimates of Lemma 5.2

$$\sum_{(t)} \sigma_i \le \sum_{(6)} \sigma_i + \sum_{(6)} \sigma_i + \sum_{(6)} \sigma_i + \sum_{(t-18)} \sigma_i$$

$$< -1.52\,pt - 1.52\,pt - 1.52\,pt + (26 - 18)\,pt < 3.5\,pt.$$

Similarly, if we have the pattern $(6, 6, 4)$, then we find

$$\sum_{(t)} \sigma_i \leq -1.52\,pt - 1.52\,pt + 0.33\,pt + (26 - 16)\,pt < 8\,pt.$$

(Proof of 5.1.7): We use the same method as in the proof of 5.1.6. If we have the pattern $(6, 6)$, and if $t \leq 22$, then

$$\sum_{(t)} \sigma_i \leq \sum_{(6)} \sigma_i + \sum_{(6)} \sigma_i + \sum_{(t-12)} \sigma_i \leq -1.52\,pt - 1.52\,pt + (22 - 12)\,pt < 8\,pt.$$

Similarly, if we have the pattern $(6, 4, 4)$, then $\sum_{(t)} \sigma_i$ is less than $-1.52\,pt + 0.33\,pt + 0.33\,pt + 8\,pt < 8\,pt$.

(Proof of 5.1.8): Let the two adjacent degree six vertices be v_1 and v_2. Let the third be v_3. The six triangles in the hexagon around v_3 give less than $-1.52\,pt$. The ten triangles in the hexagons around v_1 and v_2 give at most

$$\sum_{(4)} \sigma_i + \sum_{(6)} \sigma_i < 1.5\,pt - 1.52\,pt < 0\,pt,$$

by the argument described in the case $t = 26$ of 5.1.2 (see Lemma 5.2).

Suppose that $t \leq 24$. There remain at most $24 - 16 = 8$ triangles, and they give a combined score of at most $8\,pt$. The total score is then less than $(-1.52 + 8)\,pt$, as desired.

Now assume that $t = 26$. Suppose there is a vertex v that is not adjacent to any of v_1, v_2, or v_3. As in the proof of 5.1.8, the ten triangles in the two overlapping hexagons give less than $0\,pt$. The other hexagon gives less than $-1.52\,pt$. By Lemma 5.2, the n triangles around v fall short of n points by at least $(5 - 4.52)\,pt = 0.48\,pt$. Each of the remaining triangles gives at most $1\,pt$. The score is then less than $(0 - 1.52 + (26 - 16) - 0.48)\,pt = 8\,pt$, as desired.

(Proof of 5.1.9): This follows directly from the construction of the triangulation and the close-neighbor restrictions on the lengths of the edges of a quasi-regular tetrahedron. The lengths are between $0.8 < 2\arcsin(1/2.51)$ and $2\arcsin(2.51/4) < 1.36$. This completes the proof of the proposition. ∎

Section 6. Combinatorics

Theorem 6.1. Suppose that a triangulation satisfies Proposition 4.2 and Properties 1–9 of Proposition 5.1. Then it must the triangulation of Diagram 6.2 with 14
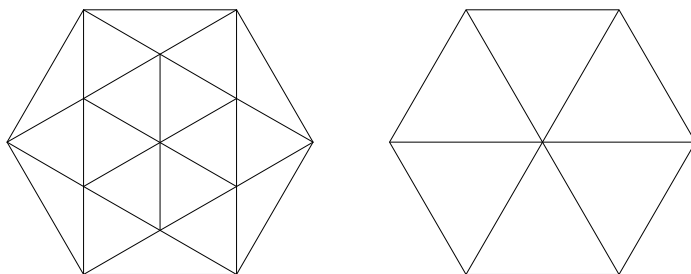
Diagram 6.2

Proof: Fix a polygon centered at a vertex u_0, such as the hexagon in Diagram 6.3. The six vertices $v_1, \ldots, v_6$ of the hexagon are distinct, for otherwise two distinct geodesic arcs on the sphere would run between u_0 and v_i for some i. This is impossible, because u_0 and v_i are not antipodal by Property 5.1.9. Similarly, the vertices of every other polygon of the triangulation are distinct.

Diagram 6.3
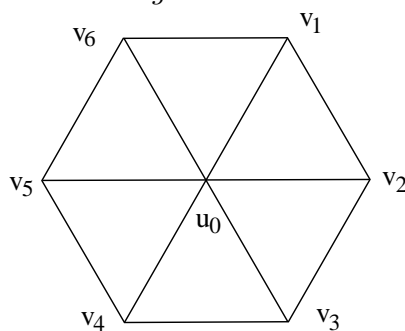
We then extend the polygon to a second layer of triangles. Each of the vertices v_i has degree four, five, or six, and two degree four vertices cannot be adjacent. The new vertices are denoted $w_1, \ldots, w_k$. One example is shown in Diagram 6.4.

Diagram 6.4
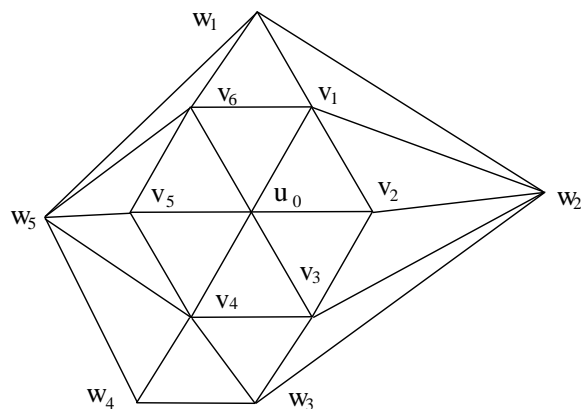
There can be no identification of a vertex v_i with a vertex w_j, for otherwise there is a triangle (say with vertices $w_j, v_k, u_0, v_i = w_j$) that is subtriangulated, contrary to Property 5.1.3. Similarly, there is no identification of two vertices w_i and w_j, for otherwise it can be checked that there is a quadrilateral (with vertices $w_i, v_k, u_0, v_\ell, w_j = w_i$) that encloses more than one vertex, which is impossible by Proposition 4.2. A purely combinatorial problem remains. It is solved in the appendix. ∎

Proposition 6.5. The triangulation of Theorem 6.1 scores less than $8\,pt$.

Proof: Our initial bound on the score comes by viewing the triangulation as made up of two hexagons and twelve additional triangles. By Lemma 5.2 and Calculation 9.1,

$$(6.6) \qquad \sum_{(24)} \sigma_i \leq \sum_{(6)} \sigma_i + \sum_{(6)} \sigma_i + \sum_{(12)} pt < -1.52\,pt - 1.52\,pt + 12\,pt = 8.96\,pt.$$

A refinement is required in order to lower the upper bound to $8\,pt$.

If a vertex v has height $|v| \geq 2.2$, then by Calculation 9.2, we find $\sigma_i < 0.5\,pt$ for the tetrahedra at v. Thus, in the Inequality 6.6, if the vertex v of some pentagon has height $|v| \geq 2.2$, then the term $\sum_{(12)} pt$ may be replaced by $\sum_{(9)} pt + \sum_{(3)} 0.5\,pt$ (there are three triangles in the pentagon that do not belong to the hexagon), and the upper bound on the score falls to $7.46\,pt$.

If a vertex of degree six has height $|v| \geq 2.05$, then we claim that $\sum_{(6)} \sigma_i < -3.04\,pt$. In fact, by Calculation 9.7, the hexagon gives

$$\sum_{(6)} \sigma_i < \sum_{(6)} (0.389195\,\mathrm{dih}(S_i) - 0.435643) = 2\pi(0.389195) - 6(0.435643) < -3.04\,pt.$$

Estimate 6.6 is improved to

$$\sum_{(24)} \sigma_i < -3.04\,pt - 1.52\,pt + 12\,pt = 7.44\,pt.$$

If the twelve tetrahedra have combined solid angle less than 6.48, then by Calculation 9.9,

$$\sum_{(12)} \sigma_i < \sum_{(12)} (0.446634\,\mathrm{sol}(S_i) - 0.190249)$$
$$\leq 6.48(0.446634) + 12(-0.190249) < 11.039\,pt.$$

Then Estimate 6.6 is improved to the bound $-1.52\,pt - 1.52\,pt + 11.039\,pt = 7.999\,pt$.

Now assume, on the other hand, that the combined solid angle of the two hexagons is at most $4\pi-6.48$. Set $K = (4\pi-6.48)/12$ and define $\sigma'(S) := \sigma(S)+(K-\text{sol}(S))/3$. The solid angle of one of the two hexagons is at most $6K$. For that hexagon, we have

$$\sum_{(6)} \sigma'(S_i) = \sum_{(6)} \sigma_i + (6K - \sum_{(6)} \text{sol}(S_i))/3 \geq \sum_{(6)} \sigma_i.$$

By our previous estimates, we now assume without loss of generality that the heights $|v|$ of the vertices of triangles in the hexagon are at most 2.05, 2.2, and 2.2, the bound of 2.05 occurring at the center of the hexagon. By Calculation 9.15,

$$\sum_{(6)} \sigma'(S_i) \leq \sum_{(6)} 0.564978\,\text{dih}_i - 0.614725 = 2\pi(0.564978)+6(-0.614725) < -2.5\ pt.$$

Estimate 6.6 becomes

$$\sum_{(24)} \sigma_i \leq \sum_{(6)} \sigma'(S_i) + \sum_{(6)} \sigma_i + \sum_{(12)} \sigma_i < (-2.5 - 1.52 + 12)\ pt = 7.98\ pt.$$

This completes the proof of the proposition. ∎

Section 7. The Method of Subdivision

The rest of this paper is devoted to the verification of the inequalities that have been used in Sections 5 and 6. In this section we describe the method used to obtain several of our bounds. We call it the method of subdivision. Let $p(x) = \sum_I c_I x^I$ be a polynomial with real coefficients c_I, where $I = (i_1, \ldots, i_n)$, $x = (x_1, \ldots, x_n) \in \mathbb{R}^n$, and $x^I = x_1^{i_1} \cdots x_n^{i_n}$. It is clear that if C is the product of intervals $[a_1, b_1] \times \cdots \times [a_n, b_n] \subset \mathbb{R}^n$ in the positive orthant ($a_i > 0$, for $i = 1, \ldots, n$), then

$$\forall x \in C, \qquad p_{\min}(C) \leq p(x) \leq p_{\max}(C),$$

where

$$p_{\min}(C) = \sum_{c_I > 0} c_I a^I + \sum_{c_I < 0} c_I b^I \quad \text{and} \quad p_{\max}(C) = \sum_{c_I > 0} c_I b^I + \sum_{c_I < 0} c_I a^I.$$

Another bound comes from the Taylor polynomial $p(x) = \sum d_I (x-a)^I$ at a:

$$(7.1) \qquad d_0 + \sum_{d_I < 0, I \neq 0} d_I (b-a)^I \leq p(x) \leq d_0 + \sum_{d_I > 0, I \neq 0} d_I (b-a)^I.$$

If $r(x) = p(x)/q(x)$ is a rational function, and if $q_{\min}(C) > 0$, then

$$\forall x \in C, \qquad \frac{p_{\min}(C)}{q_1(C, p)} \leq r(x) \leq \frac{p_{\max}(C)}{q_2(C, p)},$$

where $q_1(C,p)$ (resp. $q_2(C,p)$) is defined as $q_{\max}(C)$ whenever $p_{\min}(C) \geq 0$ (resp. $p_{\max}(C) < 0$) and as $q_{\min}(C)$ otherwise.

Let us define a *cell* to be a product of intervals in the positive orthant of $\mathbb{R}^n$. By covering a region with a sufficiently fine collection of cells, various inequalities of rational functions are easily established. To prove an inequality of rational functions with positive denominators (say $r_1(x) < r_2(x)$, for all $x \in C$), we cover C with a finite number of cells and compare the upper bound of $r_1(x)$ with the lower bound of $r_2(x)$ on each cell. If it turns out that some of the cells give too coarse a bound, then we subdivide each of the delinquent cells into a number of smaller cells and repeat the process. If at some stage we succeed in covering the original region C with cells on which the upper bound of $r_1(x)$ is less than the lower bound of $r_2(x)$, the inequality is established.

A refinement of this approach applies the method to the partial derivatives. If, for instance, we establish by the method of subdivision that for some i

$$\frac{\partial p}{\partial x_i}(x) \geq 0, \qquad \forall x \in C,$$

then we may compute an upper bound of p by applying the method of subdivision to the polynomial obtained from p by the specialization $x_i = b_i$, where b_i is the upper bound of x_i on C. Thus, we obtain an upper bound on a polynomial by fixing all the variables that are known to have partial derivatives of fixed sign and then applying the method subdivision to the resulting polynomial. Similar considerations apply to lower bounds and to rational functions with positive denominators.

It is a fortunate circumstance that many of the polynomials we encounter in sphere packings are quadratic in each variable with negative leading coefficient (u, ρ, Δ, χ in the next section). In this case, the lower bound is attained at a corner of the cell. Of course, the maximum of a quadratic function with negative leading coefficient is also elementary: $-\alpha(x - x_0)^2 + \beta \leq \beta$, if $\alpha \geq 0$.

## Section 8. Explicit Formulas for Compression, Volume, and Angle

Many of the formulas in this section are classical. One can typically find them in nineteenth century primers on solid geometry. The formula for solid angles, for example, is due to Euler and Lagrange. For anyone equipped with symbolic algebra software, the verifications are elementary, so we omit many of the details. All formulas in this section will be valid for Delaunay simplices and for quasi-regular tetrahedra, unless otherwise noted.

8.1. The Volume of a Simplex

As in the previous section, a *cell* in $\mathbb{R}^n$ is a product of intervals in $\mathbb{R}^n$. We define a function $\Delta : [4, 16]^6 \subset \mathbb{R}^6 \to \mathbb{R}$ by

$$\Delta(x_1, \ldots, x_6) = x_1 x_4(-x_1 + x_2 + x_3 - x_4 + x_5 + x_6)$$
$$+ x_2 x_5(x_1 - x_2 + x_3 + x_4 - x_5 + x_6)$$
$$+ x_3 x_6(x_1 + x_2 - x_3 + x_4 + x_5 - x_6)$$
$$\text{(8.1.1)} \qquad - x_2 x_3 x_4 - x_1 x_3 x_5 - x_1 x_2 x_6 - x_4 x_5 x_6.$$

We set $y_i = \sqrt{x_i}$, for $i = 1, \ldots, 6$. This relationship between x_i and y_i remains in force to the end of the paper. Index the edges of a simplex as in Diagram 8.1.2.

Diagram 8.1.2
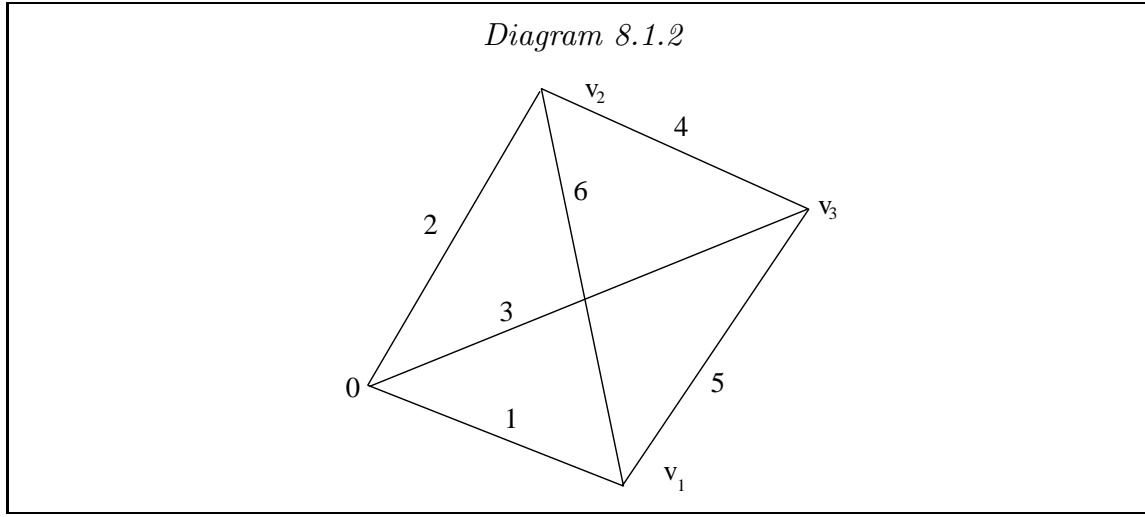
We also define $u : [4, 16]^3 \to \mathbb{R}$ by

$$u(x_1, x_2, x_6) = (y_1 + y_2 + y_6)(y_1 + y_2 - y_6)(y_1 - y_2 + y_6)(-y_1 + y_2 + y_6)$$
$$\text{(8.1.3)} \qquad = -x_1^2 - x_2^2 - x_6^2 + 2x_1 x_6 + 2x_1 x_2 + 2x_2 x_6.$$

Lemma 8.1.4. There exists a simplex of positive volume with edges of length $y_1, \ldots, y_6$ if and only if $\Delta(x_1, \ldots, x_6) > 0$. If these conditions hold, then the simplex has volume $\Delta(x_1, \ldots, x_6)^{\frac{1}{2}}/12$.

Proof: The function $u = u(x_1, x_2, x_6)$ is quadratic in each variable, with negative leading coefficient, so the minimum of u, which is 0, is attained at a vertex of the cube $[4, 16]^3$. At the vertices where the minimum is attained, $\Delta(x_1, \ldots, x_6) \leq 0$.

Assume $\Delta > 0$. Then $u > 0$, and a simplex exists with vertices 0, $X = (y_1, 0, 0)$, $Y = \frac{1}{2}(*, u^{\frac{1}{2}}/y_1, 0)$, $Z = (*, *, (\Delta/u)^{\frac{1}{2}})$. Conversely, if the simplex exists, then it must be of the given form, up to an orthogonal transformation, so $u > 0$ (otherwise O, X, and Y are colinear) and $\Delta > 0$. The volume is $|\det(X, Y, Z)|/6 = \Delta^{\frac{1}{2}}/12$. ∎

Let C be a cell contained in $[4, 16]^6$. The minimum of Δ on C is attained at a vertex

coefficient. To obtain an upper bound on Δ on a cell, we may use the method of Section 7. The restriction of Δ to the zero set of $\partial\Delta/\partial x_1$ is

$$\frac{u(x_4, x_5, x_6) \cdot u(x_2, x_3, x_4)}{4x_4}.$$

This is an upper bound on $\Delta(x_1, \dots, x_6)$.

8.2. The Circumradius of a Simplex

The circumradius of a face with edges y_4, y_5, and y_6 is

$$\eta(y_4, y_5, y_6) = \frac{y_4 y_5 y_6}{u(y_4^2, y_5^2, y_6^2)^{1/2}}.$$

Define $\rho : [4, 16]^6 \to \mathbb{R}$ by

(8.2.1) $\rho(x_1, \dots, x_6) = -x_1^2 x_4^2 - x_2^2 x_5^2 - x_3^2 x_6^2 + 2x_1 x_2 x_4 x_5 + 2x_1 x_3 x_4 x_6 + 2x_2 x_3 x_5 x_6.$

Lemma 8.2.2. Suppose $\Delta > 0$; then $\rho > 0$.

Proof: If $\Delta > 0$, then the simplex of Lemma 8.1.4 exists. Let the coordinates of the circumcenter of the simplex be (x, y, z). Direct calculation shows that $0 < x^2 + y^2 + z^2 = \rho/(4\Delta)$. ∎

Corollary 8.2.3. Let S be a Delaunay simplex of positive volume with edges of lengths $y_i = \sqrt{x_i}$. The circumradius is $\frac{1}{2}(\rho/\Delta)^{\frac{1}{2}}$.

Set

$$\chi(x_1, x_2, x_3, x_4, x_5, x_6) = x_1 x_4 x_5 + x_1 x_6 x_4 + x_2 x_6 x_5 + x_2 x_4 x_5 + x_5 x_3 x_6$$
$$+ x_3 x_4 x_6 - 2x_5 x_6 x_4 - x_1 x_4^2 - x_2 x_5^2 - x_3 x_6^2.$$

We have

$$\frac{\rho}{4\Delta} - \eta(y_4, y_5, y_6)^2 = \frac{\chi(x_1, \dots, x_6)^2}{4u(x_4, x_5, x_6)\Delta}.$$

The vanishing of χ is the condition for the circumcenter of the simplex to lie in the plane through the face T bounded by the fourth, fifth, and sixth edges. χ is positive if the circumcenter of S and the vertex of S opposite T lie on the same side of the plane through T and negative if they lie on opposite sides of the plane. We will say that T has *positive orientation* when $\chi > 0$.

8.2.4. The function ρ is quadratic in each of the variables $x_1, \dots, x_6$ with negative

The derivative is $\Delta^2 \partial(\rho/\Delta)/\partial x_1 = \chi(x_5, x_6, x_1, x_2, x_3, x_4)\chi(x_1, x_2, x_3, x_4, x_5, x_6)$. This leads to bounds on the circumradius by the method of Section 7.

The circumradius of a quasi-regular tetrahedron is increasing in $x_1, \ldots, x_6$ if the orientation of each face is positive. When a face fails to have positive orientation, it satisfies the constraints of Section 3 (for example $y_1, y_2, y_3 \in [2, 2.15]$, $y_4, y_5, y_6 \in [2.3, 2.51]$, $\eta(y_4, y_5, y_6) \geq \sqrt{2}$, if it is the face opposite the origin). This allows us to determine bounds on the circumradius for most of the quasi-regular tetrahedra we encounter in this paper by inspection. For example, in Section 9 we will study the simplices constrained by $y_i \in [2, 2.1]$. An upper bound on the circumradius is $\mathrm{rad}(S(2.1, 2.1, 2.1, 2.1, 2.1, 2.1))$.

8.2.5. Proof of Lemma 3.4. In the notation of Section 3.4, let T be the given face, and let v_0 be a vertex satisfying the conditions of the lemma. Let S be the simplex at the origin $v_0 = 0$, whose first, second, and third edges abut at v_i, for $i = 1, 2, 3$. Suppose for a contradiction that $|v_0 - v_3|^2 = x_3 \geq 2.15^2$. In light of the results of this section, a contradiction follows if $\chi(x_1, \ldots, x_6) > 0$, for $x_i \geq 4$ for $i = 1, 2$, $x_3 \geq 2.15^2$, $2.3^2 \leq x_i \leq 2.51^2$ for $i = 4, 5, 6$. (The lower bound of 2.3 comes from Remarks 3.2 and 3.3: the circumradius of T is at least $\sqrt{2}$). Since T is acute,

$$\frac{\partial \chi}{\partial x_1} = x_4(-x_4 + x_5 + x_6) > 0.$$

Similarly, χ is increasing in x_2 and x_3. Thus, to minimize χ, we take $x_1 = x_2 = 4$, $x_3 = 2.15^2$. But χ is quadratic in each variable x_4, x_5, and x_6 with negative leading coefficient, so the minimum occurs at a corner point of $[2.3^2, 2.51^2]^3$. We find $\chi \geq \chi(2^2, 2^2, 2.15^2, 2.51^2, 2.51^2, 2.51^2) \approx 0.885 > 0$. ∎

For the set of Delaunay stars to be a compact topological space, simplices of zero volume must be included. Since the circumradius remains bounded, the degenerate Delaunay simplices of zero volume are planar quadrilaterals that possess a circumscribing circle.

8.3. Dihedral Angles

Let $\mathrm{dih}(S)$ be the dihedral angle of a simplex S along the first edge. It is the (interior) angle formed by faces with edges $(2, 1, 6)$ and $(1, 3, 5)$.

Lemma 8.3.1.

$$\cos \mathrm{dih}(S) = \frac{\partial \Delta/\partial x_4}{(u(x_1, x_2, x_6)u(x_1, x_3, x_5))^{1/2}},$$

where u is the function defined by Equation 8.1.3.

The partial derivative of $\cos \text{dih}(S)$ with respect to x_3 is

$$\frac{2x_1(\partial\Delta/\partial x_2)}{u(x_1, x_2, x_6)^{1/2}u(x_1, x_3, x_5)^{3/2}},$$

so that the sign of the partial derivative is determined by the sign of $\partial\Delta/\partial x_2$. Similar considerations apply to the partial derivatives with respect to x_2, x_5, and x_6.

Lemma 8.3.2. Let S be a quasi-regular tetrahedron. Then the dihedral angle of S along the any edge is at most $\arccos\left(\frac{-29003}{96999}\right) = \text{dih}_{\max} \approx 1.874444$.

Proof: Suppose that $\text{dih}(S) > \pi/2$, so that the numerator $n = \partial\Delta/\partial x_4$ in Lemma 8.3.1 is negative. To bound $\cos \text{dih}(S)$ from below, we minimize $u(x_1, x_2, x_6)$, $u(x_1, x_3, x_5)$, and the numerator n over the variables x_2, x_3, x_5, and x_6.

We have $\partial_i u = x_j + x_k - x_i > 0$ on the indicated domain, for $i = 2, 3, 5$, and 6, so that
$$u(x_1, x_2, x_6)u(x_1, x_3, x_5) \geq u(x_1, 2^2, 2^2)^2 = (-x_1^2 + 16x_1)^2.$$

Similarly $\partial_i n = x_1 + x_j - x_k > 0$, for $i = 2, 3, 5$, and 6, so that

$$n(x_1, \ldots, x_6) > n(x_1, 2^2, 2^2, x_4, 2^2, 2^2) = x_1(16 - x_1 - 2x_4).$$

Thus,

$$0 \geq \cos \text{dih}(S) \geq \frac{16 - x_1 - 2x_4}{16 - x_1} = 1 - \frac{2x_4}{16 - x_1} \geq 1 - \frac{2(2.51)^2}{16 - 2.51^2} = \frac{-29003}{96999}.$$

∎

8.4. The Solid Angles of a Delaunay Simplex

Let S be a Delaunay simplex with vertices $v_0, \ldots, v_3$. By the solid angle $\text{sol}_i(S)$ of the simplex at the vertex i, we mean $3\text{vol}(S \cap B_i)$, where B_i is a unit ball centered at v_i. For simplicity, suppose that v_0 is located at the origin, and that in the notation of Diagram 8.1.2, the vertices v_1, v_2, v_3 are the edges of lengths y_1, y_2, and y_3. We write sol for sol_0. Set
(8.4.1)
$$a(y_1, y_2, \ldots, y_6) = y_1 y_2 y_3 + \frac{1}{2}y_1(y_2^2 + y_3^2 - y_4^2) + \frac{1}{2}y_2(y_1^2 + y_3^2 - y_5^2) + \frac{1}{2}y_3(y_1^2 + y_2^2 - y_6^2).$$

Lemma 8.4.2.
$$\text{sol}(S) = 2\arccot(\frac{2a}{\Delta^{1/2}}).$$

Proof: (See [H2, p.64]). We use the branch of arccot taking values in $[0, \pi]$. ∎

The function a is increasing in y_1, y_2, and y_3 on $[2, 4]$ and is decreasing in the variables y_4, y_5, and y_6 on the same interval.

We claim that $a > 0$ for any Delaunay simplex. We will prove this in the case $\Delta > 0$, leaving the degenerate case $\Delta = 0$ to the reader. The area of the face T opposite the origin is at most $4\sqrt{3}$ (since its edges are all at most 4). There exists a plane that is tangent to the unit sphere between this face and the unit sphere [H1,2.1]. The area of the radial projection of T to the this plane is less than the area of a disk D of radius 1.5 on the plane centered at the point of tangency. The solid angle (that is, the area of the radial projection of T to the unit sphere) is less than the area of the radial projection of D to the unit sphere. This area is $2\pi(1 - \cos(\arctan(1.5))) < \pi$. Lemma 8.4.2 now gives the result. This allows us to use Lemma 8.4.2 in the form $\mathrm{sol}(S) = 2\arctan(\Delta^{1/2}/(2a))$.

8.4.3. The solid angle is the area of a spherical triangle. Let x, y, and z be the cosines of the radian lengths of the edges of the triangle. By the spherical law of cosines, the solid angle, expressed as a function of x, y, and z is

$$c(x, y, z) + c(y, z, x) + c(z, x, y) - \pi, \quad c(x, y, z) := \arccos\left(\frac{x - yz}{\sqrt{(1 - y^2)(1 - z^2)}}\right).$$

The partial derivative with respect to x of this expression for the solid angle is $(-1 - x + y + z)/((x+1)\sqrt{t})$, where $t = 1 - x^2 - y^2 - z^2 + 2xyz$. The second derivative of this expression evaluated at $-1 - x + y + z = 0$ is $-2(1-y)(1-z)t^{-3/2} \leq 0$. So the unique critical point is always a local maximum. If neither edge at a vertex of a spherical triangle is constrained, then the triangle can be contracted or expanded by moving the vertex. If the lengths of the edges are constrained to lie in a product of intervals, then the minimum area occurs when two of the edges are as short as possible and the third is at one of the extremes. The maximum area is attained when two of the edges are as long as possible and the third is at one of the extremes or at a critical point: $x = y + z - 1$ (or it symmetries, $y = x + z - 1$, $z = x + y - 1$).

8.5. The Compression of a Delaunay Simplex

The compression $\Gamma(S)$ of a Delaunay simplex S is defined as

$$(8.5.1) \qquad \Gamma(S) = -\delta_{oct}\mathrm{vol}(S) + \sum_{i=1}^{4} \mathrm{sol}_i(S)/3,$$

where

$$(8.5.2) \qquad \delta_{oct} = \frac{-3\pi + 12\arccos(1/\sqrt{3})}{\quad} \approx 0.72.$$

We let $a_0 = a(y_1, y_2, y_3, y_4, y_5, y_6)$, where a is the function defined in 8.4.1. We also let a_1, a_2, and a_3 be the functions a for the vertices denoted v_1, v_2, and v_3 in Diagram 8.1.2. For example, $a_1 = a(y_1, y_5, y_6, y_4, y_2, y_3)$. Set $t = \sqrt{\Delta}/2$. By the results of Sections 8.1 and 8.4, we find that $\Gamma(S) = -\delta_{oct} t/6 + \sum_0^3 (2/3) \arctan(t/a_i)$. Recall that $a_i > 0$ on a cell C. We wish to give an elementary upper bound of Γ on C. Set, for $t \geq 0$ and $a = (a_0, a_1, a_2, a_3) \in \mathbb{R}_+^4$,

$$\gamma(t, a) := \frac{-\delta_{oct} t}{6} + \sum_{i=0}^3 \frac{2}{3} \arctan\left(\frac{t}{a_i}\right).$$

The partial derivative of γ with respect to a_i is $-2t/(3(t^2 + a_i^2)) \leq 0$, so $\gamma(t, a) \leq \gamma(t, a^-)$, where $a^- = (a_0^-, a_1^-, a_2^-, a_3^-)$ is a lower bound of a on C, as determined by Section 8.4. We study $\gamma(t) = \gamma(t, a^-)$ as a function of t to obtain an upper bound on $\Gamma(S)$. We note that

$$\gamma'(t) = \frac{-\delta_{oct}}{6} + \frac{2}{3} \sum_{i=0}^3 \frac{a_i}{(t^2 + a_i^2)} \quad \text{and} \quad \gamma''(t) = -\frac{4}{3} \sum \frac{a_i t}{(t^2 + a_i^2)^2} \leq 0.$$

Upper and lower bounds on t are known from Section 8.1. An upper bound on γ for t in $[t_{\min}, t_{\max}]$ is the maximum of $\ell(t_{\min})$ and $\ell(t_{\max})$, where ℓ is the tangent to γ at any point in $[t_{\min}, t_{\max}]$.

8.6. Voronoi cells

We assume in this section that the simplex S has the property that the circumcenter of each of the three faces with vertex at the origin lies in the cone at the origin over the face. This condition is automatically satisfied if these three faces are acute triangles. In particular, it is satisfied for a quasi-regular tetrahedron.

When the cone over a quasi-regular tetrahedron S contains the circumcenter of S, Section 2 sets $\mathrm{vor}(S) = -4\delta_{oct}\mathrm{vol}(\hat{S}_0) + 4\,\mathrm{sol}(S)/3$, where $\hat{S}_0$ is the intersection of S with a Voronoi cell at the origin. Otherwise, $\mathrm{vor}(S)$ is defined as an analytic continuation. This section gives formulas for $\mathrm{vol}(\hat{S}_0)$.

As usual, set $S = S(y_1, \ldots, y_6)$ and $x_i = y_i^2$. Suppose at first that the circumcenter of S is contained in the cone over S. The polyhedron $\hat{S}_0$ breaks into six pieces, called the *Rogers simplices*. A Rogers simplex is the convex hull of the origin, the midpoint of an edge (the first, second or third edge), the circumcenter of a face along the given edge, and the circumcenter of S. Each Rogers simplex has the form

$$R = R(a, b, c) := S(a, b, c, (c^2 - b^2)^{1/2}, (c^2 - a^2)^{1/2}, (b^2 - a^2)^{1/2})$$

for some $1 \leq a \leq b \leq c$. Here a is the half-length of an edge, b is the circumradius of a face, and c is the circumradius of the Delaunay simplex.

The volume is $\mathrm{vol}(R(a, b, c)) = a(b^2 - a^2)^{1/2}(c^2 - b^2)^{1/2}/6$. The density $\delta(a, b, c)$ of $R = R(a, b, c)$ is defined as the ratio of the volume of the intersection of R with a unit ball at the origin to the volume of R. It follows from the definitions that

$$(8.6.1) \qquad \mathrm{vor}(S) = \sum 4\mathrm{vol}(R(a, b, c))(-\delta_{oct} + \delta(a, b, c)),$$

where c is the circumradius $\mathrm{rad}(S)$, and (a, b) runs over the six pairs

$$(y_1/2, \eta(y_1, y_2, y_6)), \quad (y_2/2, \eta(y_1, y_2, y_6)),$$
$$(y_2/2, \eta(y_2, y_3, y_4)), \quad (y_3/2, \eta(y_2, y_3, y_4)),$$
$$(y_3/2, \eta(y_3, y_1, y_5)), \quad (y_1/2, \eta(y_3, y_1, y_5)).$$

Upper and lower bounds on $\mathrm{vol}(R(a, b, c))$ follow without difficulty from upper and lower bounds on a, b, and c. Thus, an upper bound on $\delta(a, b, c)$ leads to an upper bound on $\mathrm{vor}(S)$. The next lemma, which is due to Rogers, gives a good upper bound [R].

Lemma 8.6.2. The density $\delta(a, b, c)$ is monotonically decreasing in each variable for $1 < a < b < c$.

Proof: Let $1 \leq a_1 \leq b_1 \leq c_1$, $1 \leq a_2 \leq b_2 \leq c_2$, $a_2 \leq a_1$, $b_2 \leq b_1$, $c_2 \leq c_1$. The points of $R(a_1, b_1, c_1)$ are realized geometrically by linear combinations

$$\mathbf{s}_1 = \lambda_1(a_1, 0, 0) + \lambda_2(a_1, (b_1^2 - a_1^2)^{1/2}, 0) + \lambda_3(a_1, (b_1^2 - a_1^2)^{1/2}, (c_1^2 - b_1^2)^{1/2}),$$

where $\lambda_1, \lambda_2, \lambda_3 \geq 0$ and $\lambda_1 + \lambda_2 + \lambda_3 \leq 1$. The points of $R(a_2, b_2, c_2)$ are realized geometrically by linear combinations

$$\mathbf{s}_2 = \lambda_1(a_2, 0, 0) + \lambda_2(a_2, (b_2^2 - a_2^2)^{1/2}, 0) + \lambda_3(a_2, (b_2^2 - a_2^2)^{1/2}, (c_2^2 - b_2^2)^{1/2}),$$

with the same restrictions on λ_i. Then

$$|\mathbf{s}_1|^2 - |\mathbf{s}_2|^2 = \lambda_1(\lambda_1 + 2\lambda_2 + 2\lambda_3)(a_1^2 - a_2^2) + \lambda_2(\lambda_2 + 2\lambda_3)(b_1^2 - b_2^2) + \lambda_3^2(c_1^2 - c_2^2).$$

So $|\mathbf{s}_1|^2 \geq |\mathbf{s}_2|^2$. This means that the linear transformation $\mathbf{s}_1 \mapsto \mathbf{s}_2$ that carries the simplex S_1 to S_2 moves points of the simplex S_1 closer to the origin. In particular, the linear transformation carries the part in S_1 of the unit ball at the origin into the unit ball. This means that the density of $R(a_1, b_1, c_1)$ is at most that of $R(a_2, b_2, c_2)$. ∎

If the circumcenter of S is not in the cone over S, then the analytic continuation gives

$$\mathrm{vor}(S) = \sum 4\epsilon_R \mathrm{vol}(R(a, b, c))(-\delta_{oct} + \delta(a, b, c)),$$

where $\epsilon_R = 1$ if the face of the Delaunay simplex S corresponding to R has positive orientation, and $\epsilon_R = -1$ otherwise. (The face of S "corresponding" to $R(a, b, c)$ is the one used to compute the circumradius b.)

8.6.3. A calculation based on the explicit coordinates of S and its circumcenter given in 8.1.4 shows that

$$\epsilon_R \text{vol}(R(y_1/2, \eta(y_1, y_2, y_6), \text{rad}(S))) = \frac{x_1(x_2 + x_6 - x_1)\chi(x_4, x_5, x_3, x_1, x_2, x_6)}{48u(x_1, x_2, x_6)\Delta(x_1, \ldots, x_6)^{1/2}}.$$

If the circumcenter of S is not contained in S, then the same formula holds by analytic continuation. By definition, $\epsilon_R = -1$ exactly when the function χ is negative. Although this formula is more explicit than the earlier formula, it tends to give weaker estimates of $\text{vor}(S)$ and was not used in the calculations in Section 9.

8.6.4. There is another approximation to $\text{vor}(S)$ that will be useful. Set $S_y = S(2, 2, 2, y, y, y)$. (We hope there is no confusion with the previous notation S_i.) For $1 \leq a \leq b \leq c$, let $\text{vol}(R(a, b, c)) = a((b^2 - a^2)(c^2 - b^2))^{1/2}/6$ be as above. Set $r(a) = \text{vol}(R(a, \eta(2, 2, 2a), 1.41))$.

Lemma 8.6.5. Assume that the circumradius of a quasi-regular tetrahedron S is at least 1.41, and that $6 \leq y_1 + y_2 + y_3 \leq 6.3$. Set $a = (y_1 + y_2 + y_3 - 4)/2$. Pick y to satisfy $\text{sol}(S_y) = \text{sol}(S)$. Then

$$\text{vor}(S) \leq \text{vor}(S_y) - 8\delta_{oct}(1 - 1/a^3)r(a)$$

Proof: If S is any quasi-regular tetrahedron, let S_{tan} be the simplex defining the "tangent" Voronoi cell, that is, S_{tan} is the simplex with the same origin that cuts out the same spherical triangle as S on the unit sphere, but that satisfies $y_1 = y_2 = y_3 = 2$. The lengths of the fourth, fifth, and sixth edges of S_{tan} are between $\sqrt{8 - 2(2.3)} = \sqrt{3.4}$ and 2.51. The faces of S_{tan} are acute triangles. A calculation similar to the proof in 8.2.5, based on $\chi(3.4, 3.4, 4, 4, 4, 2.51^2) > 0$, shows that the circumcenter of S_{tan} is contained in the cone over S_{tan}.

Since S_{tan} is obtained by "truncating" S, we observe that $\text{vor}(S) = \text{vor}(S_{\text{tan}}) - 4\delta_{oct}\text{vol}(\hat{S}\backslash\hat{S}_{\text{tan}})$, where $\hat{S}$ and $\hat{S}_{\text{tan}}$ are the pieces of Voronoi cells denoted $\hat{S}_0$ in Section 2 for S and S_{tan}, respectively. By a convexity result of L. Fejes Tóth, $\text{vor}(S_{\text{tan}}) \leq \text{vor}(S_y)$ [FT,p.125]. (This inequality relies on the fact that the circumcenter of S_{tan} is contained in the cone over S_{tan}.)

Let a_1 be the half-length of the first, second, or third edge. Since $\text{vol}(R(a_1, b, c))$ is increasing in c, we obtain a lower bound on $\text{vol}(R(a_1, b, c))$ for $c = 1.41$, the lower

bound on the circumradius of S. The function $\text{vol}(R(a_1, b, 1.41))$, considered as a function of b, has at most one critical point in $[a_1, 1.41]$ and it is always a local maximum (by a second derivative test). Thus,

$$(8.6.6) \qquad \text{vol}(R(a_1, b, c)) \geq \min(\text{vol}(R(a_1, b_{\min}, 1.41)), \text{vol}(R(a_1, b_{\max}, 1.41))),$$

where $b_{\min}$ and $b_{\max}$ are upper and lower bounds on $b \in [a_1, 1.41]$. A lower bound on b is $\eta(2, 2, 2a_1)$, which means that $\text{vol}(R(a_1, b_{\min}, 1.41))$ may be replaced with $r(a_1)$ in the Inequality 8.6.6. By Heron's formula, the function $\eta(a, b, c)$, for acute triangles, is convex in pairs of variables:

$$\eta_{aa}\eta_{bb} - \eta_{ab}^2 = \frac{\eta^6(a^2 + b^2 - c^2)(a^2 - b^2 + c^2)(-a^2 + b^2 + c^2)(a^2 + b^2 + c^2)}{a^6 b^6 c^4} > 0.$$

Thus, an upper bound on $b_{\max}$ is $\eta(2, 2.51, 2a)$, where $a = (y_1 + y_2 + y_3 - 4)/2$. This means that

$$\text{vol}(R((a_1, b_{\max}, 1.41)))$$

may be replaced with the function $\text{vol}(R(a_1, \eta(2, 2.51, 2a), 1.41))$ in the Inequality 8.6.6. Now $1 \leq a_1 \leq a$, and $\text{vol}(R(a_1, b, c))$ is decreasing in the first variable (for $1 \leq a_1$ and $b \leq \sqrt{2}$), so we may use the lower bound

$$\text{vol}(R(a, \eta(2, 2.51, 2a), 1.41))$$

instead. By Calculations 9.20.2 and 9.20.3, we conclude that $\text{vol}(R(a_1, b, c)) \geq r(a)$. This lower bound is valid for each Rogers simplex. The volume of $\hat{S}\backslash\hat{S}_{\tan}$ is then at least

$$((1 - 8/y_1^3) + (1 - 8/y_2^3) + (1 - 8/y_3^3))2r(a).$$

The concavity of $1 - 8/y^3$ gives $\sum_{i=1}^{3}(1 - 8/y_i^3) \geq 1 - 1/a^3$. We have established that

$$\text{vol}(\hat{S}\backslash\hat{S}_{\tan}) \geq (1 - 1/a^3)2r(a).$$

The result follows. ∎

8.6.7. We conclude our discussion of Voronoi cells with a few additional comments about the case in which analytic continuation is used to define $\text{vor}(S)$, with S a quasi-regular tetrahedron. Assume the circumcenter c of S lies outside S and that the face T of S with negative orientation is the one bounded by the first, second, and sixth edges. It follows from Section 3 that $y_1, y_2, y_6 \in [2.3, 2.51]$ and $y_3, y_4, y_5 \in [2, 2.15]$.

Let p_1 (resp. p_2) be the point on T equidistant from the origin, v_3, and v_1 (resp. v_2).

$$|p_1|^2 = \frac{x_1}{4} + \frac{x_1 u(x_1, x_2, x_6)(-x_1 + x_3 + x_5)^2}{4(\partial\Delta/\partial x_4)^2}.$$

Diagram 8.6.8
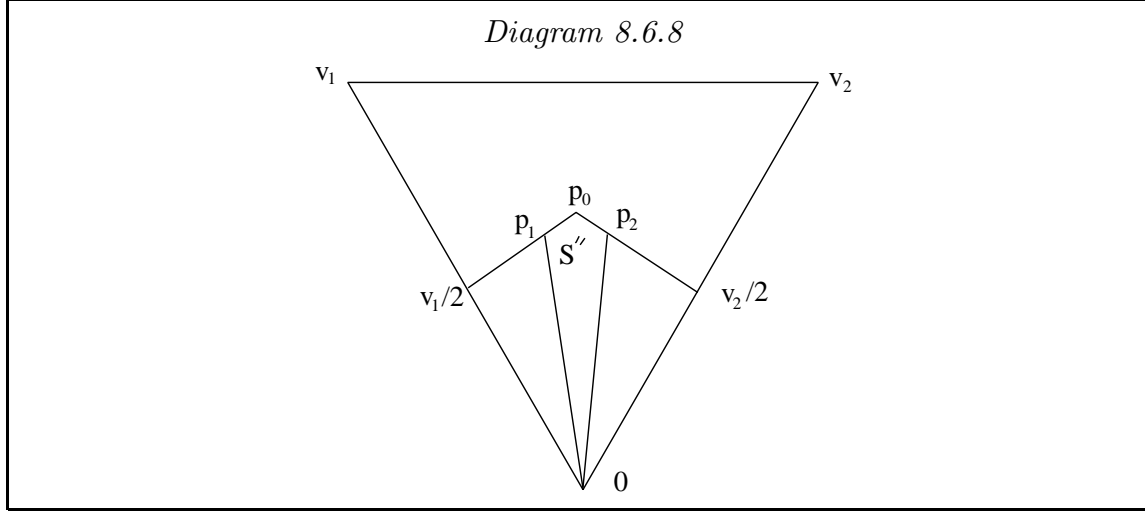
$\epsilon_R = -1$ for the Rogers simplex with vertices the origin, p_0, c and $v_1/2$. It lies outside S. The other Rogers simplex along the first edge has $\epsilon_R = 1$, so that the part common to both of these Rogers simplices cancels in the definition of $\mathrm{vor}(S)$. This means that $\mathrm{vor}(S)$ becomes the sum of the usual contributions from the two Rogers simplices along the third edge,

$$4\mathrm{vol}(R(a,b,c))(-\delta_{oct} + \delta(a,b,c))$$

for $(a,b,c) = (y_1/2, \eta(y_1, y_3, y_5), |p_1|))$ and $(y_2/2, \eta(y_2, y_3, y_4), |p_2|)$, and

$$v(S'') := 4\delta_{oct}\mathrm{vol}(S'') - 4\,\mathrm{sol}(S'')/3,$$

where S'' is the convex hull of 0, p_0, p_1, p_2, and c.

We claim that in any cell satisfying the constraints given above, $|p_1|$ is minimized by making y_1, y_2, y_6 as large as possible and y_3, y_4, y_5 as small as possible. To show this, one has to write out the derivatives explicitly from the formula for $|p_1|^2$ given above. The partial derivatives with respect to $x_2, \dots, x_6$ factor into products of the polynomials $\partial\Delta/\partial x_i$, for $i = 3, 4, 5$, x_1, $(x_3 + x_5 - x_1)$, $u(x_1, x_2, x_6)$, $(-x_1 x_4 + x_2 x_5 + x_1 x_6 - x_5 x_6)$, and $(x_1 x_2 - x_2 x_3 - x_1 x_4 + x_3 x_6)$. The signs of these polynomials are easily determined. The partial with respect to x_1 is complicated (the numerator has 88 terms), and we had to resort to the method of subdivision to determine its sign. We omit the details.

To complete our estimate, we describe an upper bound on $v(S'')$. The ratio $\mathrm{sol}(S'')/(3\mathrm{vol}(S''))$ is at least $1/\mathrm{rad}(S)^3$, because S'' is contained in a sphere of radius $\mathrm{rad}(S)$, centered at the origin. We have

$$\frac{\mathrm{vol}(S'')}{2} \leq \frac{1}{6}|p_0 - p_1|\,|c - p_0|\,|p_0|,$$

because the convex hull of $0, p_0, p_1$, and c, which is one side of S'', is a pyramid

course, $|c - p_0|^2 = \text{rad}(S)^2 - \eta(y_1, y_2, y_6)^2$. We now have a bound on $v(S'')$ in terms of quantities that have been studied in Section 8, if we rely on the bound $|p_0 - p_1| \leq 0.1381$. Write $p_1 = p_1(y_1, \ldots, y_6)$. This bound is obtained from the following inequalities.

$$
\begin{aligned}
|p_0 - p_1| &= (\eta(y_1, y_2, y_6)^2 - x_1/4)^{1/2} - (|p_1|^2 - x_1/4)^{1/2} \\
&\leq (\eta(y_1, 2.51, 2.51)^2 - x_1/4)^{1/2} - (|p_1(y_1, 2.51, 2, 2, 2, 2.51)|^2 - x_1/4)^{1/2} \\
&\leq (\eta(2.51, 2.51, 2.51)^2 - 2.51^2/4)^{1/2} - \\
&\qquad (|p_1(2.51, 2.51, 2, 2, 2, 2.51)|^2 - 2.51^2/4)^{1/2} \\
&< 0.1381.
\end{aligned}
$$

The inequality that replaces y_1 with 2.51 results from Calculation 9.21.

8.7. A Final Reduction

Let S be a Delaunay simplex. Suppose that the lengths of the edges y_1, y_5, and y_6 are greater than 2. Let S' be a simplex formed by contracting the vertex joining edges 1, 5, and 6 along the first edge by a small amount. We assume that the lengths y_1', y_5', and y_6' of the new edges are still at least 2 and that the circumradius of S' is at most 2, so that S' is a Delaunay simplex.

Proposition 8.7.1. $\Gamma(S') > \Gamma(S)$.

We write sol_i, for $i = 1, 2, 3$, for the solid angles at the three vertices p_1, p_2, and p_3 of S terminating the edges 1, 2, and 3. Let p_1' be the vertex terminating edge 1 of S'. Similarly, we write sol_i', for $i = 1, 2, 3$, for the solid angles at the corresponding vertices of S'. We set $\text{vol}(V) = \text{vol}(S) - \text{vol}(S')$ and $w_i = \text{sol}_i - \text{sol}_i'$. It follows directly from the construction of S' that w_2 and w_3 are positive. The dihedral angle α along the first edge is the same for S and S'. The angle β_i of the triangle $(0, p_1, p_i)$ at p_1 is less than the angle β_i' of the triangle $(0, p_1', p_i)$ at p_1', for $i = 2, 3$. It follows that w_1 is negative, since $-w_1$ is the area of the quadrilateral region of Diagram 8.7.2 on the unit sphere.

Diagram 8.7.2
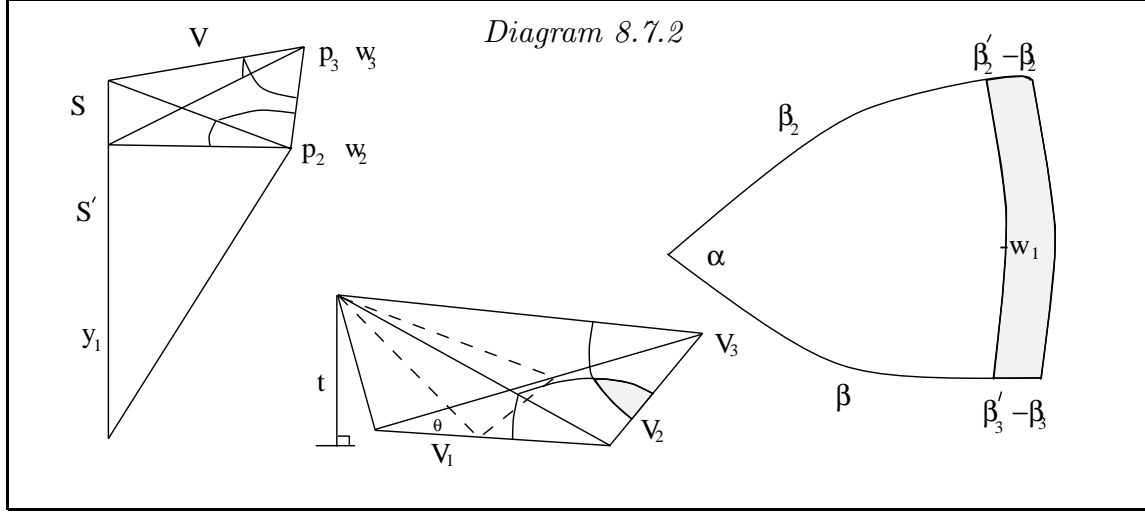
Lemma 8.7.3. $\delta_{oct}\mathrm{vol}(V) > w_2/3 + w_3/3$.

The lemma immediately implies the proposition because $w_1 < 0$ and

$$\Gamma(S') - \Gamma(S) = -w_1/3 - w_2/3 - w_3/3 + \delta_{oct}\mathrm{vol}(V).$$

Proof: Let T' be the face of S' with vertices p_1', p_2, and p_3. We consider S' as a function of t, where t is the distance from p_1 to the plane containing T'. (See Diagram 8.7.2.) It is enough to establish the lemma for t infinitesimal.

As shown in Diagram 8.7.2, let V_1 be the pyramid formed by intersecting V with the plane through p_1 that meets the fifth edge at distance $t_0 = 1.15$ from p_3 and the sixth edge at distance t_0 from p_2. Also, let the intersection of V with a ball of radius t_0 centered at p_i be denoted V_i, for $i = 2, 3$. For t sufficiently small, the region V_1 is (essentially) disjoint from V_2 and V_3.

We claim that $\mathrm{vol}(V_1) > \mathrm{vol}(V_2 \cap V_3)$. Let θ be the angle of T' subtended by the fifth and sixth edges of S'. Then $\mathrm{vol}(V_1) = Bt/3$, where B is the area of the intersection of V_1 and T':

(8.7.4) $$B = \sin\theta(y_5' - t_0)(y_6' - t_0)/2.$$

Since S' is a Delaunay simplex, the estimates $\pi/6 \le \theta \le 2\pi/3$ from [H1,2.3] hold. In particular, $\sin\theta \ge 0.5$, so $B \ge 0.25(2 - 1.15)^2$, and $\mathrm{vol}(V_1) > 0.06\,t$.

If $\mathrm{vol}(V_2 \cap V_3)$ is nonempty, the fourth edge of S must have length less than $2t_0$. The dihedral angle α' of V along the fourth edge is then less than the tangent of

the angle, which is at most $t + O(t^2)$, in Landau's notation. As in [H1,5], we obtain the estimate

$$\mathrm{vol}(V_2 \cap V_3) \leq \alpha' \int_1^{t_0} t_0^2 - t^2 \, dt = \frac{(t_0 - 1)^2 (2t_0 + 1)\alpha'}{3} < 0.025 \, t + O(t^2).$$

This establishes the claim.

Thus, for t sufficiently small

$$\delta_{oct} \mathrm{vol}(V) \geq \delta_{oct}(\mathrm{vol}(V_1) + \mathrm{vol}(V_2) + \mathrm{vol}(V_3) - \mathrm{vol}(V_2 \cap V_3))$$
$$> (\delta_{oct} t_0^3) \left(\frac{w_2}{3} + \frac{w_3}{3} \right) > 1.09 \left(\frac{w_2}{3} + \frac{w_3}{3} \right).$$

∎

Section 9. Floating-Point Calculations

This section describes various inequalities that have been established by the method of subdivision on SUN workstations. The full source code (in C++) for these calculations is available [H6].

Floating-point operations on computers are subject to round-off errors, making many machine computations unreliable. Methods of interval arithmetic give users control over round-off errors [Int]. These methods may be reliably implemented on machines that allow arithmetic with directed rounding, for example those conforming to the IEEE/ANSI standard 754 [W],[IEEE], [NR].

Interval arithmetic produces an interval in the real line that is guaranteed to contain the result of an arithmetic operation. As the round-off errors accumulate, the interval grows wider, and the correct answer remains trapped in the interval. Apart from the risk of compiler errors and defective hardware, a bound established by interval arithmetic is as reliable as a result established by integer arithmetic on a computer. We have used interval arithmetic wherever computer precision is a potential issue (Calculations 9.1 – 9.19, in particular).

Every inequality of this section has been reduced to a finite number of inequalities of the form $r(x_0) < 0$, where r is a rational function of $x \in \mathbb{R}^n$ and x_0 is a given element in $\mathbb{R}^n$. To evaluate each rational expression, interval arithmetic is used to obtain an interval Y containing $r(x_0)$. The stronger inequality, $y < 0$ for all $y \in Y$, which may be verified by computer, implies that $r(x_0) < 0$.

To reduce the calculations to rational expressions $r(x_0)$, rational approximations to the functions $\sqrt{x}$, $\arctan(x)$, and $\arccos(x)$ with explicit error bounds are required. These were obtained from [CA]. Reliable approximations to various constants (such

as π, $\sqrt{2}$, and δ_{oct}) with explicit error bounds are also required. These were obtained in *Mathematica* and were double checked against *Maple*.

Let $S = S(y_1, \ldots, y_6)$ be a quasi-regular tetrahedron. We label the indices as in Diagram 8.1.2. Let $\Gamma = \Gamma(S(y_1, \ldots, y_6))$ be the compression. We also let dih $=$ dih$(S(y_1, \ldots, y_6))$ be the dihedral angle along the first edge, and let sol $=$ sol$(S(y_1, \ldots, y_6))$ be the solid angle at the origin, that is, the solid angle formed by the first, second, and third edges (y_1, y_2, y_3) of S.

All of the following inequalities are to be considered as inequalities of analytic functions of $y_1, \ldots, y_6$. Although each of the calculations is expressed as an inequality between functions of six variables, Lemma 8.7.1 has been invoked repeatedly to reduce the number of variables to three or four. For instance, suppose that we wish to establish $I(\text{sol}, \Gamma) < 0$, where $I(\text{sol}, \Gamma)$ is an expression in $\Gamma(S(y_1, \ldots, y_6))$ and sol$(S(y_1, \ldots, y_6))$. Invoking 8.7.1 three times, we may assume that the vertices marked v_1, v_2, and v_3 in Diagram 8.1.2 each terminate an edge of minimal length. It is then sufficient to establish the inequality in seven situations of smaller dimension; that is, we may assume the edges $i \in I$ have minimal length, where I is one of

$$\{1, 4\}, \ \{2, 5\}, \ \{3, 6\}, \ \{4, 5\}, \ \{4, 6\}, \ \{5, 6\}, \ \{1, 2, 3\}.$$

Similarly, for an inequality in Γ and dihedral angle, we reduce to the seven cases

$$I = \{1, 4\}, \ \{2, 5\}, \ \{3, 6\}, \ \{1, 2, 3\}, \ \{1, 5, 6\}, \ \{3, 4, 5\}, \ \{2, 4, 6\}.$$

The first two calculations are inequalities of the compression Γ of a quasi-regular tetrahedron.

Calculation 9.1. $\Gamma \leq 1 \, pt.$

This first inequality and Calculation 9.3 are the only ones that are not strict inequalities. Set $S_0 = S(2, 2, 2, 2, 2, 2)$. By definition, $\Gamma(S_0) = 1 \, pt$. We must give a direct proof that S_0 gives the maximum in an explicit neighborhood. Then we use the method of subdivision to bound Γ away from $1 \, pt$ outside the given neighborhood. An infinitesimal version of the following result is proved in [H1].

Lemma 9.1.1. If $y_i \in [2, 2.06]$, for $i = 1, \ldots, 6$, then $\Gamma(S(y_1, \ldots, y_6)) \leq \Gamma(S_0)$, with equality if and only if $S(y_1, \ldots, y_6) = S_0$.

Set $a_{00} = a(2, 2, 2, 2, 2, 2) = 20$, $\Delta_0 = \Delta(2^2, 2^2, 2^2, 2^2, 2^2, 2^2)$, $t_0 = \sqrt{\Delta_0}/2 = 4\sqrt{2}$, and $b_0 = (2/3)(1 + t_0^2/a_{00}^2)^{-1} = 50/81$. Set $f = \max_i(y_i - 2) \leq 0.06$ and $a^- =$

We have $\arctan(x) \le \arctan(x_0) + (x - x_0)/(1 + x_0^2)$, if $x, x_0 \ge 0$. We will verify below that $\Delta \ge \Delta_0$ under the restrictions given above. Then

$$\Gamma(S) = -\frac{\delta_{oct} t}{6} + \frac{2}{3} \sum_{i=0}^{3} \arctan(t/a_i)$$

$$\le \Gamma(S_0) - \frac{\delta_{oct}(t - t_0)}{6} + b_0 \sum_{i=0}^{3} \left(\frac{t}{a_i} - \frac{t_0}{a_{00}} \right)$$

$$= \Gamma(S_0) - \frac{\delta_{oct}(\Delta - \Delta_0)}{24(t + t_0)} + b_0 \sum_{i=0}^{3} \frac{t - t_0}{a_i}$$

$$+ \frac{b_0 t_0}{a_{00}^2} \sum_{i=0}^{3} (a_{00} - a_i) + \frac{b_0 t_0}{a_0^2} \sum_{i=0}^{3} \frac{(a_{00} - a_i)^2}{a_i}$$

$$\le \Gamma(S_0) + \frac{(\Delta - \Delta_0)}{t + t_0} \left(-\frac{\delta_{oct}}{24} + \frac{b_0}{a^-} \right) + \frac{b_0 t_0}{a_{00}^2} \sum_{i=0}^{3} (a_{00} - a_i)$$

$$(9.1.2) \qquad + \frac{b_0 t_0}{a_0^2 a^-} \sum_{i=0}^{3} (a_{00} - a_i)^2.$$

Set $c_0 = -\delta_{oct}/24 + b_0/a^- > 0$. Write $y_i = 2 + f_i$, with $0 \le f_i \le f$. Set $x_i = 4 + e_i = y_i^2 = 4 + 4f_i + f_i^2$. Then $f_i \le e_i/4$, for $i = 1, \dots, 6$. Set $e = 4f + f^2$. Set $\tilde{\Delta}(e_1, \dots, e_6) = \Delta(x_1, \dots, x_6)$. We find that $\partial^2 \tilde{\Delta}/\partial e_2 \partial e_1 = 4 + e_4 + e_5 - e_6 > 0$ and similarly that $\partial^2 \tilde{\Delta}/\partial e_i \partial e_1 > 0$, for $i = 3, 5, 6$. So $\partial \tilde{\Delta}/\partial e_1$ is minimized by taking $e_2 = e_3 = e_5 = e_6 = 0$, and this partial derivative is at least

$$\frac{\partial \tilde{\Delta}}{\partial e_1}(e_1, 0, 0, e_4, 0, 0) = 16 - 8e_1 - 2e_1 e_4 - e_4^2 \ge 16 - 8e - 3e^2 > 0.$$

Thus $\Delta \ge \Delta_0$. The partial derivative $\partial \tilde{\Delta}/\partial e_1$ is at most

$$\frac{\partial \tilde{\Delta}}{\partial e_1}(e_1, e, e, e_4, e, e) = 16 + 16e - 8e_1 + 4ee_4 - 2e_1 e_4 - e_4^2 \le 16 + 16e + 4ee_4 - e_4^2$$

$$\le 16 + 16e + 3e^2.$$

So $\Delta - \Delta_0 \le (16 + 16e + 3e^2)(e_1 + \cdots + e_6)$.

We expand $\sum_{i=0}^{3}(a_i - a_{00}) = 5(e_1 + \cdots + e_6) + h_1 + h_2 + h_3$ as a sum of homogeneous polynomials h_i of degree i in $f_1, \dots, f_6$. A calculation shows that $h_1 = 0$. Also h_2 is quadratic in each variable f_i with negative leading coefficient, so h_2 attains its minimum at an extreme point of the cube $[0, f]^6$. A calculation then shows that $h_2 \ge -14f^2$ on $[0, f]^6$. By discarding all the positive terms of h_3, we find that

$$h_3 \ge -f_1^2 f_4 - f_1 f_4^2 - f_2^2 f_5 - f_2 f_5^2 - f_3^2 f_6 - f_3 f_6^2 \ge -6f^3.$$

Thus, $\sum_{i=0}^{3}(a_i - a_{00}) \geq 5(e_1 + \cdots + e_6) - 14f^2 - 6f^3$. Since $e = \max(e_i)$, we find that $f \leq e/4 \leq (e_1 + \cdots + e_6)/4$. This gives

$$\sum_{i=0}^{3}(a_{00} - a_i) \leq (e_1 + \cdots + e_6)(-5 + \frac{7f}{2} + \frac{3f^2}{2}).$$

Similarly, we expand $\sum_{i=0}^{3}(a_{00} - a_i)^2$ as a polynomial in $f_1, \ldots, f_6$. To obtain an upper bound, we discard all the negative terms of the polynomial and evaluate all the positive terms at $(f_1, \ldots, f_6) = (f, \ldots, f)$. This gives

$$\sum_{i=0}^{3}(a_{00} - a_i)^2 \leq 4944f^2 + 7296f^3 + 3684f^4 + 828f^5 + 73f^6$$

$$\leq \frac{1}{4}(e_1 + \cdots + e_6)(4944f + 7296f^2 + 3684f^3 + 828f^4 + 73f^5).$$

We now insert these estimates back into Inequality 9.1.2. This gives

$$\frac{\Gamma(S) - \Gamma(S_0)}{(e_1 + \cdots + e_6)} \leq \frac{c_0}{2t_0}(16 + 16e + 3e^2) + \frac{b_0 t_0}{a_{00}^2}(-5 + 3.5f + 1.5f^2)$$

(9.1.3)
$$+ \frac{b_0 t_0}{4a_{00}^2 a^-}(4944f + 7296f^2 + 3684f^3 + 828f^4 + 73f^5).$$

The right-hand side of this inequality is a rational function of f. (Both a^- and e depend on f.) Each of the three terms on the right-hand side is increasing in f. Therefore, the right-hand side reaches its maximum at $f = 0.06$. Direct evaluation at $f = 0.06$ gives $\Gamma(S) - \Gamma(S_0) \leq -0.00156(e_1 + \cdots + e_6)$. ∎

To verify Calculation 9.14, the computer examined only 7 cells. Calculation 9.1 required 1,899 cells. Calculation 9.6.1 required over 2 million cells. The number of cells required in the verification of the other inequalities falls between these extremes.

Calculation 9.2. $\Gamma < 0.5 \, pt$, if $y_1 \in [2.2, 2.51]$.

The next several calculations are concerned with the relationship between the dihedral angle and the compression.

Calculation 9.3.

$$\mathrm{dih}(S(y_1, \ldots, y_6)) \geq \mathrm{dih}_{\min} := \mathrm{dih}(S(2, 2.51, 2, 2, 2.51, 2)) \approx 0.8639.$$

Since this bound is realized by a simplex, we must carry out the appropriate local

Lemma 9.3.1. Suppose that $2 \leq y_i \leq 2.2$, for $i = 1, 3, 6$, and that $2 \leq y_i \leq 2.51$, for $i = 2, 4, 5$. Then $\text{dih}(S(y_1, \ldots, y_6)) \geq \text{dih}_{\min}$.

Proof: This is an application of Lemma 8.3.1. By that lemma, $\text{dih}(S)$ is increasing in x_4, so we fix $x_4 = 4$. The sign of $\partial \cos \text{dih} / \partial x_2$ is the sign of $\partial \Delta / \partial x_3$, and a simple estimate based on the explicit formulas of Section 8 shows that $\partial \Delta / \partial x_3 > 0$ under the given constraints. Thus, we minimize $\text{dih}(S)$ by setting $x_2 = 2.51^2$. By symmetry, we set $x_5 = 2.51^2$.

Now consider $\text{dih}(S)$ as a function of x_1, x_3, and x_6. The sign of $\partial \cos \text{dih} / \partial x_3$ is the sign of $\partial \Delta(x_1, 2.51^2, x_3, 2^2, 2.51^2, x_6) / \partial x_2$. The maximum of this partial (about -2.39593) is attained when x_1, x_3, and x_6 are as large as possible: $x_1 = x_3 = x_6 = 2.2^2$. So $\text{dih}(S)$ is increasing in x_3. We take $x_3 = 4$, and by symmetry $x_6 = 4$.

We have
$$\frac{\partial \cos \text{dih}(S)}{\partial x_1} = \frac{2t_1(x_1)}{u(x_1, x_2, x_6)^{3/2} u(x_1, x_3, x_5)^{3/2}},$$
where $t_1(x_1) \approx 464.622 - 1865.14x_1 + 326.954x_1^2 - 92.9817x_1^3 + 4x_1^4$. An estimate of the derivative of $t_1(x)$ shows that $t_1(x)$ attains its maximum at $x_1 = 4$, and $t_1(4) < -6691 < 0$. Thus $\text{dih}(S)$ is minimized when $x_1 = 4$. ∎

Calculation 9.4. $\Gamma < 0.378979 \, \text{dih} - 0.410894$.

Lemma 9.5. If S_1, S_2, S_3, and S_4 are any four tetrahedra such that $\text{dih}(S_1) + \text{dih}(S_2) + \text{dih}(S_3) + \text{dih}(S_4) \geq 2\pi$, then $\Gamma(S_1) + \cdots + \Gamma(S_4) < 0.33 \, pt$.

This lemma is a consequence of the following three calculations, each established by interval arithmetic and the method of subdivision.

Calculation 9.5.1.
$$\Gamma < -0.19145 \, \text{dih} + 0.2910494,$$
provided $\text{dih} \in [\text{dih}(S(2, 2, 2, 2, 2, 2)), 1.42068]$.

Calculation 9.5.2.
$$\Gamma < -0.0965385 \, \text{dih} + 0.1562106,$$
provided $\text{dih} \in [1.42068, \text{dih}(S(2, 2, 2, 2.51, 2, 2))]$.

Calculation 9.5.3.
$$\Gamma < -0.19145 \, \text{dih} + 0.31004,$$
provided dih $>$ dih$(S(2, 2, 2, 2.51, 2, 2))$

To deduce Lemma 9.5, we consider the piecewise linear bound ℓ on Γ obtained from these estimates. The linear pieces are $\ell_1(x) \leq 1\,pt$, ℓ_2, ℓ_3, and ℓ_4 on $[\text{dih}_{\min}, d_1]$, $[d_1, d_2]$, $[d_2, d_3]$, and $[d_3, \text{dih}_{\max}]$, where $d_1 = \text{dih}(S(2, 2, 2, 2, 2, 2))$, $d_2 = 1.42068$, and $d_3 = \text{dih}(S(2, 2, 2, 2.51, 2, 2))$. (See Calculation 9.1, and Lemma 8.3.2.) Diagram 9.5.4 illustrates these linear bounds. (There are small discontinuities at d_1, d_2, and d_3 that may be eliminated by replacing ℓ_i by $\ell_i + \epsilon_i$, for some $\epsilon_i > 0$, for $i = 1, 2$, and 4.) We then ask for the maximum of $\ell(t_1) + \ell(t_2) + \ell(t_3) + \ell(t_4)$ under the constraint $(t_1 + t_2 + t_3 + t_4)/4 \geq \pi/2 \in [d_2, d_3]$. Since $\ell(x)$ is constant on $(\text{dih}_{\min}, d_1)$ and decreasing on $[d_1, \text{dih}_{\max}]$, we may assume that $t_i \geq d_1$, for all i. Since the slope of ℓ_2 is equal to the slope of ℓ_4, we may assume that $t_i \geq d_2$, for all i, or that $t_i \leq d_3$, for all i. If $t_i \leq d_3$, for all i, then we find that $t_i \geq 2\pi - 3d_3 > d_2$. So in either case, $t_i \geq d_2$, for all i. By convexity, an upper bound is $4\ell_3(\pi/2) < 0.33\,pt$.

Diagram 9.5.4
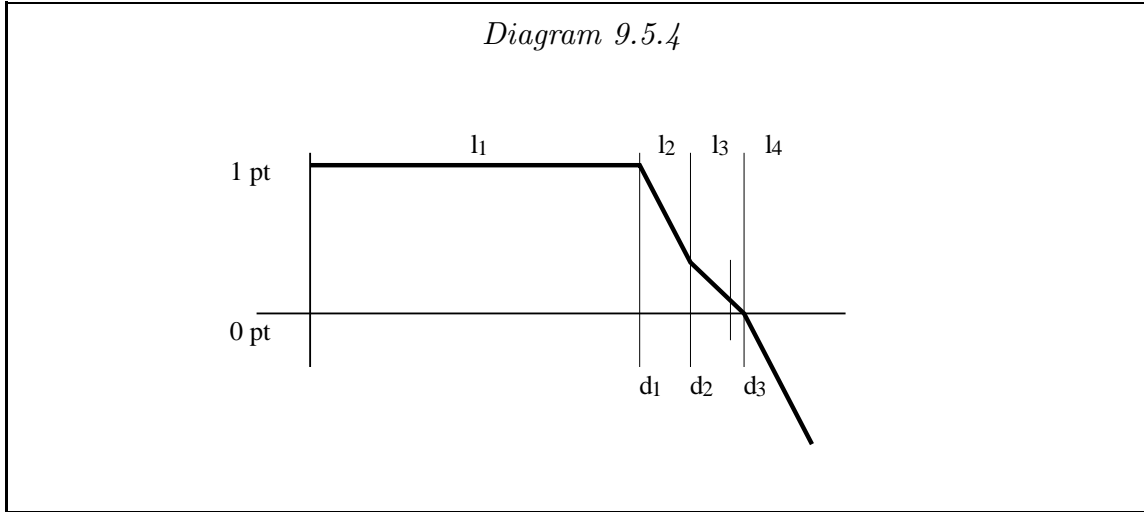
Lemma 9.6. If $S_1, \ldots, S_5$ are any five tetrahedra such that $\text{dih}(S_1) + \cdots + \text{dih}(S_5) \geq 2\pi$, then

$$\Gamma(S_1) + \cdots + \Gamma(S_5) < 4.52\,pt.$$

This is a consequence of two other calculations.

Calculation 9.6.1. $\Gamma < -0.207045\,\text{dih} + 0.31023815$, provided $\text{dih} \in [d_0, 2\pi - 4d_0]$, where $d_0 = \text{dih}(S(2, 2, 2, 2, 2, 2))$.

Calculation 9.6.2. $\Gamma < 0.028792018$, if $\text{dih} > 2\pi - 4d_0$.

Calculations 9.1, 9.6.1, and 9.6.2 give a piecewise linear bound ℓ on Γ as a function of dihedral angle. See Diagram 9.6.3. (Again, there are minute discontinuities that may be eliminated in the same manner as before.) We claim that $4.52\,pt > \ell(t_1) + \cdots + \ell(t_5)$ whenever $t_1 + \cdots + t_5 \geq 2\pi$. As in Lemma 9.5, we may assume that $t_i \geq d_0$. Since ℓ is decreasing on $[d_0, \text{dih}_{\max}]$, we may assume that $t_1 + \cdots + t_5 = 2\pi$.

Thus, only the interval $[d_0, 2\pi - 4d_0]$ is relevant for the optimization. On this interval, the bound is linear, so $\ell(t_1) + \cdots + \ell(t_5) \le 5\ell(2\pi/5) < 4.52\,pt.$

Diagram 9.6.3
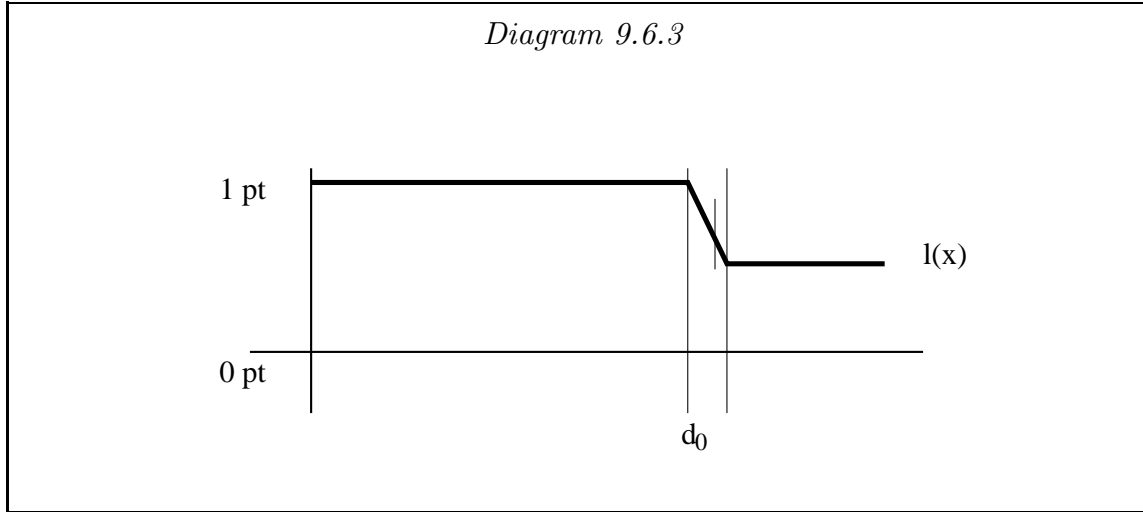
Calculation 9.7. $\Gamma < 0.389195\,\mathrm{dih} - 0.435643$, if $y_1 \ge 2.05$.

The next inequalities relate the solid angles to the compression.

Calculation 9.8. $\Gamma < -0.37642101\,\mathrm{sol} + 0.287389$.

Calculation 9.9. $\Gamma < 0.446634\,\mathrm{sol} - 0.190249$.

Calculation 9.10. $\Gamma < -0.419351\,\mathrm{sol} + 0.2856354 + 0.001$, if $y_i \in [2, 2.1]$, for $i = 1, \ldots, 6$.

The following calculation involves the circumradius. We leave it to the reader to check that the dimension-reduction techniques of Lemma 8.7.1 may still be applied.

Calculation 9.11. $\Gamma < -0.419351\,\mathrm{sol} + 0.2856354$, provided that $y_4, y_5, y_6 \ge 2.1$ and that the circumradius of S is at most 1.41.

Calculation 9.12. $\Gamma < -0.419351\,\mathrm{sol} + 0.2856354 - 5(0.001)$, if $y_i > 2.1$ for some i, and $y_4 \in [2, 2.1]$.

Calculation 9.13. $\Gamma < -0.65557\,\mathrm{sol} + 0.418$, if $y_i \in [2, 2.1]$, for $i = 1, \ldots, 6$.

Calculation 9.14. $\mathrm{sol}(S) > 0.21$.

Calculation 9.15. $\Gamma + (K - \mathrm{sol})/3 < 0.564978\,\mathrm{dih} - 0.614725$, where $K = (4\pi -$

Calculation 9.16. dih > 0.98 and sol > 0.45, provided $y_1 \in [2, 2.05]$, and $y_2, y_3 \in [2, 2.2]$.

Let $\Gamma(S)$ be replaced by vor(S) in each of the Calculations $9.1 - 9.16$ to obtain a new list of inequalities $9.1'- 9.16'$. (In $9.11'$, we drop the constraint on the circumradius of S.) We claim that all of the inequalities $9.*'$ hold whenever S is a quasi-regular tetrahedron of circumradius at least 1.41. In fact, Inequalities $9.1'$, $9.2'$, $9.4'$, $9.5.1'$, $9.5.2'$, $9.5.3'$, $9.6.1'$, $9.6.2'$, and $9.7'$ follow directly from 9.17 and the inequalities $\text{dih}_{\min} \leq \text{dih} \leq \text{dih}_{\max}$. Calculations 9.3, 9.14, and 9.16 are independent of Γ, and so do not require modification. Inequalities $9.8'$, $9.11'$, and $9.12'$ also rely on 9.17, 9.18 and 9.19, inequality $9.9'$ on 9.14, and inequality $9.15'$ on 9.16. Inequalities $9.10'$ and $9.13'$ are vacuous by the comments of $8.2.4$.

Write $S = S(y_1, y_2, y_3, y_4, y_5, y_6)$, vor $=$ vor(S), and let rad $=$ rad(S) be the circumradius of S.

Lemma 9.17. If the circumradius is at least 1.41, then vor $< -1.8\,pt$.

Proof: If sol ≥ 0.91882, then the lemma is a consequence of Lemma 9.18. (The proof of Lemma 9.18, under the restriction sol ≥ 0.91882, is independent of the proof of this lemma.) Assume that sol < 0.91882.

If S' and S are Delaunay stars, related as in Section 8.7, then vor$(S') >$ vor(S) because $\hat{S}_0'$ is obtained by slicing a slab from $\hat{S}_0$. This means that we may apply the dimension-reduction techniques described at the beginning of this section, unless the deformation decreases the circumradius to 1.41. An interval calculation establishes the result when $y_1 + y_2 + y_3 \geq 6.3$ and the circumradius constraint is met (Calculation $9.17.1$). When the dimension reduction techniques apply, the dimension of the search space may be reduced to four, and an interval calculation similar to the others in this section gives the result (Calculation $9.17.2$).

We lacked the computer resources to perform the interval analysis directly when the dimension-reduction techniques fail and found it necessary to break the problem up into smaller pieces when $y_1 + y_2 + y_3 \leq 6.3$. We will make use of the following calculations.

Calculation 9.17.1. vor$(S) < -1.8\,pt$ provided $y_1 + y_2 + y_3 \geq 6.3$, rad$(S) = 1.41$, and sol$(S) \leq 0.91882$.

Calculation 9.17.2. vor$(S) < -1.8\,pt$ provided that rad$(S) > 1.41$, $y_1 + y_2 + y_3 \geq 6.3$, sol$(S) \leq 0.912882$, and S lies in one of the seven subspaces of smaller dimension associated with $I(\text{sol}, \Gamma)$ at the beginning of the section.

Calculation 9.17.3.1. Assume that $y_1 + y_2 + y_3 \leq 6.3$ and that rad ≥ 1.41. Then sol ≥ 0.767.

Calculation 9.17.3.2. Assume that $y_1 + y_2 + y_3 \leq 6.192$ and that rad ≥ 1.41. Then sol ≥ 0.83.

Calculation 9.17.3.3. Assume that $y_1 + y_2 + y_3 \leq 6.106$ and that rad ≥ 1.41. Then sol ≥ 0.87.

Calculation 9.17.3.4. Assume that $y_1 + y_2 + y_3 \leq 6.064$ and that rad ≥ 1.41. Then sol ≥ 0.9.

Calculation 9.17.3.5. Assume that $y_1 + y_2 + y_3 \leq 6.032$ and that rad ≥ 1.41. Then sol ≥ 0.91882.

In the interval arithmetic verification of Calculations 9.17.3, we may assume that rad $= 1.41$ and that $y_1 + y_2 + y_3$ is equal to the given upper bound 6.3, 6.192, etc. To see this, we note that the circumradius constraint is preserved by a deformation of S that increases y_1, y_2, or y_3 while keeping fixed the spherical triangle on the unit sphere at the origin cut out by S. We increase y_1, y_2, and y_3 in this way until the sum equals the given upper bound. Then fixing y_1, y_2, y_3, and one of y_4, y_5, and y_6, we decrease the other two edges in such a way as to decrease the solid angle and circumradius until rad $= 1.41$.

This deformation argument would break down if we encountered a configuration in which two of y_4, y_5, and y_6 equal 2, but this cannot happen when $\mathrm{rad}(S) \geq 1.41$ because this constraint on the edges would lead to the contradiction

$$1.41 \leq \mathrm{rad}(S) \leq \mathrm{rad}(S(2.3, 2.3, 2.3, 2, 2, 2.51)) < 1.39.$$

It is possible to reduce Calculations 9.17.3 further to the four-dimensional situation where two of y_4, y_5 and y_6 are either 2 or 2.51. Consider a simplex S with vertices 0, v_1, v_2, and v_3. Let p_i be the corresponding vertices of the spherical triangle cut out by S on the unit sphere at the origin. Fix the origin, v_2, and v_3, and vary the vertex v_1. The locus on the unit sphere described as p_1 traces out spherical triangles of fixed area is an arc of a Lexell circle $\mathcal{C}$. Define the "interior" of $\mathcal{C}$ to be the points on the side of $\mathcal{C}$ corresponding to spherical triangles of smaller area. The locus traced by v_1 on the circumsphere (of S) with $|v_1|$ constant is a circle. Let $\mathcal{C}'$, also a circle, be the radial projection of this locus to the unit sphere. Define the "interior" of $\mathcal{C}'$ be the points coming from larger $|v_1|$. The two circles $\mathcal{C}$ and $\mathcal{C}'$ meet at p_1, either tangentially or transversely. The interior of $\mathcal{C}$ cannot be contained in the interior of $\mathcal{C}'$ because the Lexell arc contains p_2^*, the point on the unit sphere antipodal to p_2 [FT,p.23], but the interior of of $\mathcal{C}'$ does not. Furthermore, if $|v_1| = 2$ and $|v_2| + |v_3| > 4$, then v_2 or v_3 lies in the interior of $\mathcal{C}$ and $\mathcal{C}'$, so that the circles

have interior points in common. This means that one can always move v_1 in such a way that the solid angle is decreasing, the circumradius is constant, and the length $|v_1|$ is decreasing (or constant if $|v_1| = 2$). If any two of y_4, y_5, and y_6 are not at an extreme point, this argument can be applied to v_1, v_2, or v_3 to decrease the solid angle. This proves the reduction.

We are now in a position to prove the lemma for simplices satisfying $y_1 + y_2 + y_3 \leq 6.3$. Calculation 9.17.3.1 allows us to assume sol ≥ 0.767. As in Section 8.6, let $S_y = S(2, 2, 2, y, y, y)$. We will rely on the fact that $\mathrm{vor}(S_y)$ is decreasing in y, for $y \in [2.26, 2.41]$. In fact, the results of Section 8.6 specialize to the formula

$$(9.17.4) \qquad \mathrm{vor}(S_y) = \frac{-8\delta_{oct}y^2}{(12 - y^2)^{1/2}(16 - y^2)} + \frac{8}{3}\arctan\left(\frac{(12 - y^2)^{1/2}y^2}{64 - 6y^2}\right),$$

and the sign of its derivative is determined by a routine *Mathematica* calculation. It is clear that $\mathrm{sol}(S_y)$ is continuous and increasing in y. Since $\mathrm{sol}(S_{2.26}) < 0.767$ and $\mathrm{sol}(S_{2.41}) > 0.91882$, our conditions imply that $\mathrm{sol}(S) = \mathrm{sol}(S_y)$ for some $y \in [2.26, 2.41]$. Let $r(a)$ and $\mathrm{vol}(R(a, b, c))$ be the functions introduced in Section 8.6.4.

This suggests the following procedure. Pick y so that $\mathrm{sol}(S) \geq \mathrm{sol}(S_y)$. Calculate the smallest (or at least a reasonably small) a for which

$$\xi(y, a) := \mathrm{vor}(S_y) - 4\delta_{oct}(1 - 1/a^3)2r(a)$$

is less than $-1.8\, pt$. Monotonicity (Calculation 9.20.1) and Lemma 8.6.5 imply that $\mathrm{vor}(S) < -1.8\, pt$, if $y_1 + y_2 + y_3 \geq 2(2 + a)$. To treat the case that remains $(y_1 + y_2 + y_3 < 2(2 + a))$, use Calculations 9.17.3 to obtain a new lower bound on $\mathrm{sol}(S)$, and hence a new value for y. The procedure is repeated until $a = 0.016$. Calculation 9.17.3.5 completes the argument by covering the case $y_1 + y_2 + y_3 \leq 6.032$. We leave it to the reader to check that

$$\xi(2.2626, 1.096), \ \xi(2.326, 1.053), \ \xi(2.364, 1.032), \ \xi(2.391, 1.016)$$

are less than $-1.8\, pt$ and that

$$\mathrm{sol}(S_{2.2626}) \leq 0.767, \ \mathrm{sol}(S_{2.326}) \leq 0.83, \ \mathrm{sol}(S_{2.364}) \leq 0.87, \ \mathrm{sol}(S_{2.391}) \leq 0.9.$$

This completes the proof of Lemma 9.17. ∎

Lemma 9.18. If $\mathrm{rad}(S) \geq 1.41$, then $\mathrm{vor} < -0.419351\,\mathrm{sol} + 0.2856354$.

Proof: We adopt the notation and techniques of Lemma 9.17. If sol ≤ 0.918819, then the result follows from Lemma 9.17. (The proof of 9.17 is independent of

$-0.419351 \operatorname{sol}(S) + 0.2856354 - \operatorname{vor}(S)$. We show that $f(S)$ is positive. We will use the inequality $f(S) \geq f(S_{\tan}) + 4\delta_{oct} \operatorname{vol}(\hat{S} \backslash \hat{S}_{\tan})$ of Lemma 8.6.4. A routine calculation based on the formula 9.17.4 shows that $f(S_y)$ is increasing, for $y \in [2.4085, 2.51]$.

If sol ≥ 0.951385, then we appeal to Fejes Tóth's convexity argument described in 8.6. To justify the use of his argument, we must verify that the cone over $S_{\tan}$ contains the circumcenter of S. The first, second, and third edges have length 2, and the fourth, fifth, and sixth edges are between 2.21 and 2.51 (Calculation 9.18.2). These are stronger restrictions on the edges than in the proof of Lemma 8.6.5, so the justification there applies here as well. We observe that $\operatorname{sol}(S_{2.4366}) < 0.951385$ so that

$$f(S) \geq f(S_{\tan}) \geq f(S_y) \geq f(S_{2.4366}) \approx 0.000024 > 0,$$

where y satisfies $\operatorname{sol}(S_y) = \operatorname{sol}(S_{\tan})$. We may now assume that $0.918819 \leq \operatorname{sol} \leq 0.951385$.

Lemma 9.18.1. The combined volume of the two Rogers simplices along a common edge of a quasi-regular tetrahedron S is at least 0.01.

Proof: The combined volume is at least that of the right-circular cone of height a and base a wedge of radius $\sqrt{b^2 - a^2}$ and dihedral angle $\operatorname{dih}_{\min}$, where a is the half-length of an edge and b is a lower bound on the circumradius of a face with an edge $2a$. This gives the lower bound of

$$\frac{\pi}{3}(b^2 - a^2)a\frac{\operatorname{dih}_{\min}}{2\pi} > 0.1439(b^2 - a^2).$$

We minimize b by setting $b^2 = \eta(2, 2, 2a)^2 = 4/(4 - a^2)$. Then $b^2 - a^2 = (a^2 - 2)^2/(4 - a^2)$, which is decreasing in $a \in [1, 2.51/2]$. Thus, we obtain a lower bound on $b^2 - a^2$ by setting $a = 2.51/2$, and this gives the estimate of the lemma. ∎

We remark that $\operatorname{sol}(S_{2.4085}) < 0.918819$. If $1.15 \leq (y_1 + y_2 + y_3 - 4)/2$, then Lemma 9.18.1 and Section 8.6 give

$$f(S) \geq f(S_{2.4085}) + 4\delta_{oct}(1 - 1/1.15^3)0.01 > 0.$$

(Analytic continuation is not required here, because of the constraints on the edges in Calculation 9.18.2.) We may now assume that $y_1 + y_2 + y_3 \leq 6.3$. To continue, we need a few more calculations.

Calculation 9.18.2. If sol ≥ 0.918, then $y_4, y_5, y_6 \geq 2.21$.

Calculation 9.18.3.1. If $y_1 + y_2 + y_3 \leq 6.02$ and rad ≥ 1.41, then sol ≥ 0.928.

Calculation 9.18.3.2. If $y_1 + y_2 + y_3 \leq 6.0084$ and rad ≥ 1.41, then sol ≥ 0.933.

Calculation 9.18.3.3. If $y_1 + y_2 + y_3 \leq 6.00644$ and rad ≥ 1.41, then sol ≥ 0.942.

In the verification of these calculations, we make the same reductions as in the Calculations 9.17.3.

Adapting the procedure of Lemma 9.17 and Lemma 8.6.5, we find that a lower bound on the solid angle leads to an estimate of a constant a with the property that $f(S) > 0$ whenever $y_1 + y_2 + y_3 \geq 4 + 2a$. That is, we pick a so that $\xi_1(y, a) := f(S_y) + 8\delta_{oct}(1 - 1/a^3)r(a)$ is positive, where y is chosen so that $\text{sol}(S_y)$ is a lower bound on the solid angle. The values

$$\xi_1(2.4085, 1.01), \ \xi_1(2.4165, 1.0042), \ \xi_1(2.42086, 1.00322), \ \xi_1(2.4286, 1.0017)$$

are all positive. This yields the bound $y_1 + y_2 + y_3 \leq 6.0034$.

Assume that S satisfies $y_1 + y_2 + y_3 \leq 6.0034$ and $\text{rad}(S) \geq 1.41$. Then by Calculation 9.18.3.3, $\text{sol}(S) = \text{sol}(S_{\tan}) \geq 0.942$. Also $\text{rad}(S_{\tan}) > \text{rad}(S)/1.0017 \geq 1.41/1.0017 > 1.4076$, because rescaling $S_{\tan}$ by a factor of 1.0017 gives a simplex containing S. This means that $S_{\tan}$ satisfies the hypotheses of the following calculation. Calculation 9.18.4 completes the proof of Lemma 9.18. ∎

Calculation 9.18.4. If $\text{rad}(S_{\tan}) \geq 1.4076$ and $0.933 \leq \text{sol}(S_{\tan}) \leq 0.951385$, then $f(S_{\tan}) > 0$.

In this verification, we may assume that the fourth fifth, and sixth edges of $S_{\tan}$ are at least 2.27. for otherwise the circumradius is at most

$$\text{rad}(S(2, 2, 2, 2.27, 2.51, 2.51)) < 1.4076.$$

In the verification of 9.18.4, we also rely on the fact that

$$f_1(x_4, x_5, x_6) := f(S(2, 2, 2, \sqrt{x_4}, \sqrt{x_5}, \sqrt{x_6}))$$

is increasing in $(x_4, x_5, x_6) \in [2.27^2, 2.51^2]$. Here is a sketch justifying this fact. The details were carried out in *Mathematica* with high-precision arithmetic. The explicit formulas of Section 8.6 lead to an expression for $\partial f_1/\partial x_4$ as

$$\frac{W(x_4, x_5, x_6)(-x_4 + x_5 + x_6)}{(-16 + x_4)^2 \Delta^{3/2}},$$

where W is a polynomial in x_4, x_5, and x_6 (with 13 terms). To show that W is positive, expand it in a Taylor polynomial about $(x_4, x_5, x_6) = (2.27^2, 2.27^2, 2.27^2)$ and check that the lower bound of Inequality 7.1 is positive.

For $a \leq b \leq c$, we have $\mathrm{vol}(R(a, b, c)) = a((b^2 - a^2)(c^2 - b^2))^{1/2}/6$. The final four calculations are particularly simple (to the extent that any of these calculations are simple), since they involve a single variable. They were verified in *Mathematica* with rational arithmetic.

Calculation 9.20.1. The function $(1-1/a^3)\mathrm{vol}(R(a, \eta(2, 2, 2a), 1.41))$ is increasing on $[1, 1.15]$.

Calculation 9.20.2. The function $\mathrm{vol}(R(a, \eta(2, 2, 2a), 1.41))$ is decreasing for $a \in [1, 1.15]$.

Calculation 9.20.3. For $a \in [1, 1.15]$ we have

$$\mathrm{vol}(R(a, \eta(2, 2, 2a), 1.41)) < \mathrm{vol}(R(a, \eta(2, 2.51, 2a), 1.41)).$$

Calculation 9.21. Let $p_1 = p_1(y_1, \ldots, y_6)$ be the point in Euclidean space introduced in Section 8.6.7. For $y \in [2.3, 2.51]$,

$$\frac{d}{dy}(\eta(2.51, 2.51, y) - y^2/4)^{1/2} > -0.75 > \frac{d}{dy}(|p_1(y, 2.51, 2, 2, 2, 2.51)|^2 - y^2/4)^{1/2}.$$

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Appendix. Proof of Theorem 6.1

Douglas J. Muder

Notation and observations. Let P be a point of degree d. If we consider P to be the center of the configuration, then the *first rim* of points will be the set of d points adjacent to P, and the *second rim* will be those at distance 2 from P. Let $\delta(P)$ be the sum of the degrees of the first rim points. If $d = 6$, it is easy to see that the number of points on the second rim is $s = \delta(P) - 24$, and the total number of points of distance at most 2 from P is $\delta(P) - 17$. The second rim is thus an s-gon. This s-gon and the triangulation of the P-side of the s-gon will be referred to as the *inner graph*. The inner-graph degree of a second rim point will be called its *inner degree*. The number of second-rim points with inner degree 5 is equal to the number of degree 4 points in the first rim, and the number of second-rim points with inner degree 3 is equal to the number of degree 6 points on the first rim. All other second-rim points have inner degree 4. Points beyond the second rim will be called *extra points*. If there are no extra points, then there are at least 2 second-rim points whose degrees are equal to their inner degrees. Let $N_\Delta^i(P)$ be the number of points of degree Δ in rim i around P. Notice that if $d = 6$, then

$$\delta(P) = 30 - N_4^1(P) + N_6^1(P).$$

Further, Euler's formula gives $N - 12 = N_6 - N_4$. Putting this together with 5.1.1 and 5.1.5, we see

$$13 \leq 12 + N_6 - N_4 \leq 15$$
$$1 \leq 1 + N_4 \leq N_6 \leq 3 + N_4 \leq 5.$$

Lemma 1. *There is no triangle whose vertices all have degree six.*

Lemma 2. *Suppose $N_6 \geq 3$. Let $\mathbf{G}_6$ be the subgraph of points of degree six. Either $\mathbf{G}_6$ is three points in two components, or it is a single (open or closed) path, with no other edges.*

With these lemmas and this notation, we consider the different possible values of N_6.

$N_6 = 1$**.** This forces $N_4 = 0$. Let P be the degree 6 point. Then $\delta(P) = 30$, all 13 points are in the inner graph, and all 6 second-rim points have inner degree 4. But at least two of these second-rim points have inner degree equal to degree. Contradiction.

$N_6 = 2.$ If the two degree 6 points are adjacent, let P be either one. Now $\delta(P) = 31 - N_4^1$, and we see that there are no extra points, and all second rim points have degree 5. All but N_4^1 second rim points have inner degree less than 5, and at least two of them will have inner degree equal to degree. So $N_4 \geq N_4^1 = 2$, and $N \leq 12$. Contradiction.

If the degree six points are not adjacent, then the $(6,6)$ forces $N \geq 14$, so $N_4 = 0$. If $\delta(P)$ is either of the two degree six points, $\delta(P) = 30$, so the second rim has 6 points, all of inner degree 4, and there is one extra point. If the extra point has degree 5, it is adjacent to all but one of the second rim points. This unique second-rim point is then part of a quadrilateral, which can only be triangulated by the diagonal edge that does not include the extra point. This creates two second-rim points of degree 6, in violation of our assumptions. Therefore the extra point has degree 6, and we have 6.2.

$N_6 = 3.$ Either $\mathbf{G}_6$ is an open path or it has two components. In either case there is a $(6,6)$, so $N \geq 14$ and $N_4 = 0$ or 1.

In the first case let P be the center of the path. Now $\delta(P) = 32 - N_4^1$. We see that there are no extra points and any degree 4 point is in the first rim. The second rim has at most one point of inner degree greater than 4, and two points whose inner degrees are equal to their degrees. So there must be a point of degree 4 on the second rim. Contradiction.

In the second case 5.1.8 forces $N = 15$, hence $N_4 = 0$. If P is one of the points in the two-point component of $\mathbf{G}_6$, then $\delta(P) = 31$, so there is one extra point and 7 second-rim points. Either one or two of the second rim points is not connected to the extra point. In either case at least one of these two has degree = inner degree, which is at most 4. Contradiction.

$N_6 = 4.$ Now $\mathbf{G}_6$ is either an open or closed path of length 4. If open, then by 5.1.8, $N = 15$ and $N_4 = 1$. If P is either of the interior degree 6 points, then $\delta(P) = 32 - N_4^1$, the second rim is an $(8 - N_4^1)$-gon with N_4^1 points of inner degree at least 5 and N_4^1 extra points. We cannot have $N_4^1 = 0$, or else there would be at least two second rim points of degree 4, so $N_4^1 = 1$. This holds no matter which interior degree 6 point we started with, so the degree 4 point must be adjacent to both. It also must be adjacent to one of the other two, or else there is a $(6,6,4)$. Therefore there is a degree 6 point whose first rim degree sequence is 6/4/6/5/5/5, producing a second rim inner degree sequence of 4/3/5/3/4/4/4. The point of inner degree 5 is the fourth neighbor of the degree four point, and cannot be degree 6 without making $\mathbf{G}_6$ closed. Therefore there is an edge connecting the two points of inner degree 3. Adding this edge to the inner graph creates a hexagon with all points of "inner" degree 4, and the extra point in its interior. The extra point is connected to 5 of these points, and the sixth has degree 4. Contradiction.

If $\mathbf{G}_6$ is a closed path, then a degree 4 point Q must triangulate this quadrilateral. Using Q as the center, there are 4 first rim points and 8 second rim points. The second rim can be drawn in a square with the 4 points of inner degree 3 on the corners and the 4 points of inner degree 4 at the midpoints. There is at most one additional degree 4 point (other than Q). If it is anywhere but at one of the second-rim midpoints, a $(6, 6, 4)$ exists. The four midpoints cannot be adjacent to any additional second-rim points without creating an illegal triangle or quadrilateral. Since there can be at most one more degree 4 point, at least 3 of the 4 second-rim midpoints must be joined to the extra point(s). Two midpoints of consecutive sides can't be joined to the same extra point without forcing the corresponding corner to be degree 4, which is impossible. So there must be two extra points, and thus no degree four points other than Q. One extra point must be joined to the midpoints of each pair of parallel sides of the square. But all these edges cannot be drawn without intersecting.

$N_6 = 5$. Now $\mathbf{G}_6$ is a path of length 5, closed so that a $(6, 6, 6)$ doesn't exist. Any point in this pentagon is nonadjacent to two others, so the situation of 5.1.8 applies in 5 different ways. Let $P, Q, R \in \mathbf{G}_6$ with P and Q adjacent, but neither adjacent to R. Then there are 8 points adjacent to either P or Q, and 6 points adjacent to R, so there are exactly two common points in these two sets. In our case these two points are precisely the other two points of degree 6. This means that no point inside or outside the pentagon can be connected to more than two points of the pentagon. Thus the only possible configuration for the 15 points is to form three concentric pentagons, with $\mathbf{G}_6$ as the middle one. Prior to triangulating the inner and outer pentagons, all of their points have degree 4. Triangulating either creates more degree 6 points. Contradiction.

Proof of Lemma 1. Let P_1, P_2, and P_3 be the vertices of such a triangle. If P_j has no neighbors of degree 4, then the only possibility is $\delta(P_j) = 32$, which forces $N_5^1 = 4, N_6^1 = 2$, and $N = 15$. All second-rim points have inner degree at most 4, and there are no extra points. Therefore two second-rim points have degree and inner degree 4. Call them Q_1 and Q_2. Therefore, $N_4 \geq 2, N_6 \geq 5$, and $N_6^2 \geq 2$. Let R_1 and R_2 be second-rim points of degree 6. Each Q_k and R_ℓ must be adjacent, or else (P_j, R_ℓ, Q_k) is a $(6, 6, 4)$. But all edges from Q_j are inner-graph edges. So $Q_1 R_1 Q_2 R_2$ must be a second-rim quadrilateral, which is impossible. Thus $N_4^1(P_j) \geq 1$ for each P_j.

This forces $N_4 = 2$. At least one of the degree 4 points is adjacent to two of the P_j. One of these two, say P_1, is not adjacent to the other degree 4 point. Since $\delta(P) \leq 32$, we are left with four possible first-rim degree sequences for P_1: (1) 6/6/4/5/5/5; (2) 6/6/4/6/5/5; (3) 6/6/4/5/6/5; or (4) 6/6/4/5/5/6.

The last three possibilities are easily dealt with. Sequence (3) contains a $(6, 6, 4)$. Sequence (4) creates two 6-6-6 triangles joined at an edge. Let P_1 and P_2 be the

vertices of the edge, and P_3 and P_4 be the other vertices of the triangles. The conditions $N_4^1(P_j) \geq 1$ and $N_4 = 2$ force P_3 and P_4 to have sequence (1). In (2) we can invoke 5.1.8 with the 3 degree 6 points in the first rim. Call them R_1, R_2 and T, with R_1 adjacent to R_2. In order for the numbers to work out, there can be precisely two points which are adjacent to T as well as one of the R_j. But in (2) the center, the first rim degree 4 point, and the second rim neighbor of the first rim degree 4 point must all fit this description.

Sequence (1) is more difficult to eliminate. Let $R_1, \ldots R_6$ be the first rim points listed in the order of (1). Let $S_1, \ldots, S_7$ be the second rim points, with S_1 being adjacent to both R_1 and R_2, and S_7 having only R_1 as a first rim neighbor. There is at least one degree 6 point in the second rim—if it is at S_1, then $\delta(R_1) = 32$; if it is anywhere else we can invoke 5.1.8. In either case, $N = 15$ and there are two degree 6 points outside the first rim. These must lie in $\{S_6, S_7, S_1, S_3\}$ to avoid making a $(6, 6, 4)$ with R_1 and R_3. At most one of these points can be adjacent to R_1 (since $\delta(R_1) < 33$), so S_3 must have degree 6. Now S_3 must connect to both the degree 6 and degree 4 points in $\{S_6, S_7, S_1\}$ to avoid making a $(6, 6, 6)$ or $(6, 6, 4)$ with the center point. But S_3 has inner degree 5 and so can connect to at most one of those points. Contradiction. ∎

Proof of Lemma 2. If $\mathbf{G}_6$ has at least three points and no triangles, then there exists a $(6, 6)$ forcing $N \geq 14$. Any point in $\mathbf{G}_6$ can be adjacent to at most two others, or else either a triangle or a $(6, 6, 6)$ is created. Therefore each component is a path. There cannot be three or more components without producing a $(6, 6, 6)$. If $\mathbf{G}_6$ has two components, each of them must be a complete graph for the same reason. Since there are no triangles, both of the components must have at most two points. If there are two components with two points each, then 5.1.8 forces $N = 15$. Each component is adjacent to 8 non-$\mathbf{G}_6$ points of the original graph, and not adjacent to 3. Now 5.1.8 forces each point in the other component to be adjacent to these 3. But two points can have only two common neighbors. So the only two-component $\mathbf{G}_6$ is the one described in the lemma. ∎